

**No. 2A-1 LiNbO<sub>3</sub>, Lithium niobate***(M* = 147.846)

1a	Ferroelectricity in LiNbO <sub>3</sub> was discovered by Matthias and Remeika in 1949. History of LiNbO <sub>3</sub> : see		49Mat 89Nas	
b	phase	II	I	a)67Nii
	state	F	P	b)66Abr1
	crystal system	trigonal	trigonal	
	space group	R3c – C <sub>3v</sub> <sup>6</sup> b)	R $\bar{3}$ c – D <sub>3d</sub> <sup>6</sup> a)	
	$\Theta_f$ [°C]	1210(10)		65Nas1
	Review paper: see			89Bri
	$P_s \parallel [001]$ of hexagonal unit cell.			66Abr2
	$T_{\text{melt}} = 1253$ °C.			58Rei
	Review paper: see			89Gra1
	$\rho = 4.4640 \cdot 10^3$ kg m <sup>-3</sup> at $T = 4$ °C.			66Abr2
	Review paper: see			89Gra2
	Color: light yellow, breach by heat treatment in oxygen atmosphere.			66Nas
	Vickers hardness number: Fig. 2A-1-001.			
	Phase relation: Fig. 2A-1-002.			
	Congruent melt composition: Li <sub>2</sub> O/Nb <sub>2</sub> O <sub>5</sub> = 48.45/51.55, $\Theta_f = 1138(2)$ °C.			85OBr
	About the stoichiometry: see			89Abr
	$\Theta_f$ : Table 2A-1-001; Fig. 2A-1-003, Fig. 2A-1-004, Fig. 2A-1-005.			
	Cleavage plane: (012).			80Kam
	Phase transition under high pressure: Fig. 2A-1-006, Fig. 2A-1-007; see also			85Got
	Anomalies in optical and other physical properties at around 100 °C have been reported by many authors. The nature which gives these anomalies has not been explained, however, the experimental results indicate that the anomalies seem to be related to the nonstoichiometry of crystals.			
	See, for example			85Che, 86Eng, 87HuX, 87Gal 83Mae, 83Tat, 79Nas
	Glassy states and phases: see			85Kum
	Preparation of ilmenite structure from NaNbO <sub>3</sub> by ion exchange reaction: see			85Wei
	A summary of physical properties and crystal structure: see			90Pro
	A monograph on LiNbO <sub>3</sub> : see			89Pit
	Epitaxial growth of LiNbO <sub>3</sub> : see			
2a	Phase diagram: Fig. 2A-1-008, Fig. 2A-1-009.			
	Crystal growth: Czochralski method.			65Bal, 65Fed, 66Nas
	Czochralski growth (review paper): see			89Fra1
	Stepanov's technique (review paper): see			89Pol
	Growth of large crystals by Czochralski method: see			88Gra
	Stoichiometric single crystal growth by double crucible Czochralski method using automatic powder supply system: see			92Kit
	Growth of off-congruent single crystals by the double crucible method: see			93Fur

Preparation of off-congruent crystals by vapor transport equilibrium (VTE) method: see	92Bor
Preparation of thin films by sol-gel method: see	94Hur
Single crystal fibers by micro-pulling down method: see	94Yoo1
Periodically poled crystals by laser-heated pedestal growth: see	90Mag
Effect of an electric field on the growth of single crystals: see	91Rei
Cutting and polishing: see	89Fra2
Poling: see	89Fra3
Proton-exchange (review papers): see	89Won1, 89Won2, 89Hin1
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3a $a_{\text{hex}} = 5.1483 \text{ \AA}$ , $c_{\text{hex}} = 13.863 \text{ \AA}$ and $a_{\text{rh}} = 5.4944 \text{ \AA}$ , $\alpha = 55^\circ 52'$ at $23^\circ \text{C}$ . $a = 5.14739(8) \text{ \AA}$ , $c = 13.85614(9) \text{ \AA}$ for the stoichiometric composition, $a = 5.15052(6) \text{ \AA}$ , $c = 13.86496(3) \text{ \AA}$ for the congruent composition. Change in $c/a$ and $V$ due to hydrostatic pressure: Fig. 2A-1-006, Fig. 2A-1-007. Change in lattice constants with stoichiometry: Fig. 2A-1-010. Lattice parameters (a review paper): see Lattice parameters of epitaxial films (a review paper): see	66Abr2  86Abr  89Gra3 89Kan1
b $Z = 4$ in hexagonal unit cell, $Z = 2$ in rhombohedral unit cell. Crystal structure: Tables 2A-1-002...2A-1-006; Figs. 2A-1-009...2A-1-012. The structure of congruent composition is expressed by $[\text{Li}_{1-5x}\text{Nb}_{5x}]\text{Nb}_{1-4x}\text{O}_3$ with $x = 0.0118(7)$ , i.e. all the Li sites are occupied by $\text{Li}^+$ and $\text{Nb}^{5+}$ ions leaving vacancies at Nb sites. Crystal structure of proton-exchanged waveguides: see	66Abr2   86Abr 94Fei
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4 Thermal expansion coefficients: $\alpha_a^{(1)} = 0.154 \cdot 10^{-4} ^\circ\text{C}^{-1}$ , $\alpha_a^{(2)} = 0.053 \cdot 10^{-7} ^\circ\text{C}^{-2}$ , $\alpha_c^{(1)} = 0.075 \cdot 10^{-4} ^\circ\text{C}^{-1}$ , $\alpha_c^{(2)} = -0.077 \cdot 10^{-7} ^\circ\text{C}^{-2}$ , where $\Delta a/a = \alpha_a^{(1)} (T - T_0) + \alpha_a^{(2)} (T - T_0)^2$ , $\Delta c/c = \alpha_c^{(1)} (T - T_0) + \alpha_c^{(2)} (T - T_0)^2$ , with $T_0 = 25^\circ \text{C}$ . Fig. 2A-016, see also a review paper Thermal expansion: Figs. 2A-1-013...2A-1-019.	71Smi   89Tay
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5a Dielectric constant ( $T = \text{RT}$ ): Table 2A-1-007. Dielectric constant (ceramics): Fig. 2A-1-020, Fig. 2A-1-021. Dielectric constant (stoichiometry dependence): Fig. 2A-1-022. Dielectric constant (frequency dependence): Figs. 2A-1-023...2A-1-030. Dielectric constant in optical region: see Fig. 2A-1-080 in 9a. Dielectric constant (temperature dependence): Figs. 2A-1-031...2A-1-036. Dielectric constant (a small amount of Fe-doping): Figs. 2A-1-037...2A-1-040. Dielectric constant (thin films): Figs. 2A-1-041...2A-1-043. Dielectric constant (pressure dependence): Fig. 2A-1-044, Fig. 2A-1-045. Effect of X-ray irradiation on $\kappa_a$ , $\kappa_c$ , $\tan \delta_a$ , $\tan \delta_c$ : see $\kappa$ vs. $T$ , $\tan \delta$ vs. $T$ of eutectic composition of $\text{LiNbO}_3$ and $3\text{Li}_2\text{O} \cdot \text{Nb}_2\text{O}_5$ : see $\kappa$ vs. $T$ (amorphous thin film) at 1 kHz...1 MHz, $\kappa_{\text{max}} \approx 10^4$ at $350^\circ \text{C}$ in a heating process: see Vitreous specimens prepared by roller quenching exhibit $\kappa > 10^5$ close to the crystallization temperatures: see A review paper on dielectric constant: see	88Sin 78Sin 81Mit  77Gla 89Tom1
b Nonlinear dielectric properties: Table 2A-1-008.	
c Spontaneous polarization: $P_s = 0.71 \text{ C m}^{-2}$ . Fig. 2A-1-047, Fig. 2A-1-048.	68Wen

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Point defects and singularities of low temperature behavior of $P$ (a review paper): see		91Nov
d	Pyroelectricity: $p_3 = -8.3 \cdot 10^{-5} \text{ C K}^{-1} \text{ m}^{-2}$ (primary effect: $-9.59 \cdot 10^{-5} \text{ C K}^{-1} \text{ m}^{-2}$ , secondary effect: $1.29 \cdot 10^{-5} \text{ C K}^{-1} \text{ m}^{-2}$ ) at RT. See also Fig. 2A-1-049, Fig. 2A-1-050. Data for calculating figure of merits: see Pyroelectric coefficient (a review paper): see Point defects and singularities of low temperature behavior of $p$ (a review paper): see	80Bha 75Bee  75Bee 89Wei1 91Nov
6a	Heat capacity: $C_p = 89 \text{ J K}^{-1} \text{ mol}^{-1}$ at 100 °C. Fig. 2A-1-051. See also a review paper Thermal conductivity: Fig. 2A-1-052. See also a review paper Thermal diffusivity: Fig. 2A-1-053. See also a review paper	75Bee  89Lin1 89Lin2 89Lin3
7a	Piezoelectricity: see Table 2A-1-007 in 5a; Fig. 2A-1-054. See also review papers  Elastoelectric properties: see	89Bal, 89Cho1 82Chi
b	Electrostriction: Table 2A-1-010. See also a review paper	89Cho2
c	Third order piezoelectric constant: $e_{222} = 21 \text{ C m}^{-2}$ , $e_{333} = -21 \text{ C m}^{-2}$ . Table 2A-1-009, Table 2A-1-011.	
8a	Elastic compliance and stiffness: see Tables 2A-1-007 in 5a; Fig. 2A-1-055, Fig. 2A-1-057. Compliance (review paper): see Stiffness (review paper): see Acoustic properties: Table 2A-1-012; Fig. 2A-1-056, Fig. 2A-1-058. Velocity of ultrasonic bulk waves (review paper): see Attenuation of ultrasonic bulk waves (review paper): see Temperature dependence of the frequency of plate resonators: see Effect of $\gamma$ -irradiation: see Hypersonic attenuation: Figs. 2A-1-059...2A-1-061; see also  Surface acoustic waves (SAWs): Table 2A-1-013; Figs. 2A-1-062...2A-1-065. The 127.86° rotated $Y$ -cut $X$ propagation mode has a low bulk spurious response level as well as a high coupling coefficient. Effect of film loading: see Interaction with guided optical wave: see Interaction with semiconductor: see Velocity of SAWs (a review paper): see Attenuation of SAWs (a review paper): see SAW properties of common orientations (a review paper): see Velocity of SAWs on proton-exchanged crystals (a review paper): see Velocity of SAWs on ion-implanted crystals: see	89Tom2 89Tom3  89Pea 89Lew1 76Bur 77Sor 71She, 71Lie, 72Maj, 76Gri  76Shi 75Par1 76Lea 75Gun 89Hin2 89Lew2 89Mor 89Hin3 89Hin4, 73Lar, 75Har

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b Nonlinear elastic properties: Table 2A-1-014, Table 2A-1-015; Fig. 2A-1-066. Third order elastic constants (a review paper): see Nonlinear coupling in surface wave: see	89Cho3 77Ali
9a Refractive index: Tables 2A-1-016...2A-1-019; Figs. 2A-1-067...2A-1-076. Refractive index of wavelength dependence: discussion (a review paper): see Refractive index of wavelength dependence: tables (a review paper): see Refractive index of epitaxial films (a review paper): see $n_o = 7.2$ , $\tan \delta = 2.5 \cdot 10^{-3}$ for $f = 126...132$ GHz, $n_o = 7.2(2)$ for $\lambda = 2.3$ mm. Refractive index change in LiNbO <sub>3</sub> :Ti waveguides: see Birefringence: Table 2A-1-001; Figs. 2A-1-077...2A-1-079. $\Delta n = 1.57$ at RT for $\lambda = 2...3$ mm. Reflection: Figs. 2A-1-080...2A-1-084. Transmission: Fig. 2A-1-085. Absorption: Figs. 2A-1-086...2A-1-089, Fig. 2A-1-076. IR spectra of hydroxyl ions (review paper): see Absorption spectra of bulk LiNbO <sub>3</sub> (review paper): see Infrared absorption band caused by OH <sup>+</sup> ions in a LiNbO <sub>3</sub> :MgO:Cr crystal: see	89Kir1 89Kir2 89Kan2 70Vol 70Vin 88Fri 70Iri 89Kov1 89Kan3 88Kov
b Electrooptic effect: Table 2A-1-020; see also Table 2A-1-001 in 1b. Fig. 2A-1-090. $r_{13}^S = +7.7 \cdot 10^{-12}$ mV <sup>-1</sup> , $r_{33}^S = +28.8 \cdot 10^{-12}$ mV <sup>-1</sup> , $r_{51}^S = +18.2 \cdot 10^{-12}$ mV <sup>-1</sup> , $r_{22}^S = +3.4 \cdot 10^{-12}$ mV <sup>-1</sup> for $\lambda = 633$ nm. $r_{33}^T = 44(6) \cdot 10^{-12}$ mV <sup>-1</sup> for $\lambda = 0.7...2$ mm. $r_{22}^T = 10(2) \cdot 10^{-12}$ mV <sup>-1</sup> for $\lambda = 2.3$ mm. Electrooptical behavior of proton-exchanged optical waveguides: see Electrooptic coefficients (a review paper): see	80Kam 83Bro 70Vin 88Rot 89Kir3
c Piezooptic effect: Table 2A-1-021. $\Pi_{12} - \Pi_{11} = 1.02 \cdot 10^{-12}$ m <sup>2</sup> N <sup>-1</sup> , $\Pi_{33} - 1.12 \Pi_{13} = 0.808 \cdot 10^{-12}$ m <sup>2</sup> N <sup>-1</sup> , $\Pi_{31} - 1.12 \Pi_{11} = 0.687 \cdot 10^{-12}$ m <sup>2</sup> N <sup>-1</sup> . Table 2A-1-022.	66Spe
d Photoelastic coefficients (a review paper): see Faraday effect: Fig. 2A-1-091. Optical activity in LiNbO <sub>3</sub> : Fe induced by light illumination was discovered: see	89Wei2 88Kos
e Nonlinear optical property: $d_{22} /  d_{36}^{KDP}  = +6.5$ , $d_{31} /  d_{36}^{KDP}  = d_{15} /  d_{36}^{KDP}  = -12.3$ , $d_{33} /  d_{36}^{KDP}  = -86$ at RT for $\lambda = 1.058$ mm. Figs. 2A-1-092...2A-1-094, see also Fig. 2A-1-002 in 1b. Nonlinear millimeter wave susceptibility: $d_{33} = 5.87 \cdot 10^{-9}$ mV <sup>-1</sup> for $\lambda = 857$ mm ( $f = 35$ GHz).	69Bec, 70Mil 83Ahn
10a Raman scattering: Table 2A-1-023; Figs. 2A-1-095...2A-1-103. The difference between $c(aa)b$ and $\bar{c}(aa)b$ geometries in Raman and Rayleigh scattering has been pointed out. Raman spectra of undoped crystal (review paper): see	83Sem 89Scol

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b Brillouin scattering: Table 2A-1-024.	
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11 Conductivity: Figs. 2A-1-104...2A-1-109.	
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Proton-exchanged optical waveguides using toluic acid: see	92Loi
Channel waveguide integrated optics (a review paper): see	88Sym
Ti-diffused waveguide devices: see	88Alf
Optical waveguides produced by Ti-in-diffusion, ion exchange, ion implantation (a review paper): see	88Car
LiNbO <sub>3</sub> :Ti:Er waveguide amplifiers: see	84Bri
Optical waveguide properties of LiNbO <sub>3</sub> thin films: see	93Shi
Integrated-optic devices for optical communication: see	87Vog
Second harmonic generation for the analysis of substrates and boules: see	87Lum
Optical properties of Ag <sup>+</sup> ion implanted crystals: see	94Sha
Anomalies in the temperature dependence of optical properties of metal-doped single crystals: see	91Sha
Optical and structural properties of MeV Er-implanted crystal: see	94Fle
Increase in optical damage resistance in Sc <sub>2</sub> O <sub>3</sub> -doped crystal: see	92Yum
Construction of a narrow-band interference filter with photorefractive effect: see	94Mul
Optical mixing coefficients in LiNbO <sub>3</sub> (a review paper): see	89Cho4
Optical detection of compositional inhomogeneities in Czochralski-grown crystals: see	94Suz
Three-dimensional visualization of 180° ferroelectric domains by electrooptic effects: see	89Otk
Defect: see	74Jar
Point defects: see	89Agu
Nonstoichiometry and the defect structure: see	94Kuz
Defect formation by $\gamma$ -ray irradiation: see	89Kor
Defect chemistry of MgO-doped crystals: see	90Fen4
Characterization of dislocations in a single crystal grown by micro pulling down method: see	94Yoo1
Suggested vacancy structure models for congruent crystal: see	84Zot
OH-related defects in metal doped LiNbO <sub>3</sub> :MgO: see	90Kov
Point defects and singularities of low temperature behavior of $P_s$ and $p$ : see	91Nov
Impurity diffusion: Table 2A-1-035.	
Stark effect in LiNbO <sub>3</sub> doped with rare earth elements (a review paper): see	89Skv
Yield stress of LiNbO <sub>3</sub> (a review paper): see	89Pet
Crystal quality characterization by $\gamma$ -ray diffraction: see	86Aub
Ti site study in LiNbO <sub>3</sub> :Ti by means of $\gamma$ - $\gamma$ perturbed angular correlated PIXE-channeling technique: see	94Hau
Lattice distortion study of 1MeV Cu ion implantation by Rutherford backscattering / channeling technique: see	92Shi
Lattice sites for transition and rare-earth impurities by ion-beam channeling methods: see	92Reb1
Analysis of diffusion of various elements: see	93Bir
He ion channeling on kV <sup>19</sup> F <sup>+</sup> implanted crystals: see	94Tan
Diffusion of tritons, deuterons, and protons: see	89Gon
Electrical characterization of thin films by RF sputtering on silicon substrates: see	90Bau
Transmission electron microscope observation of plastically deformed crystal: see	91Pet

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Physical structure of thin films: see	91Ros
Growth of MgO doped single crystal fibers by a drawing down method: see	91Ogu
Lattice site of iron in Fe <sup>3+</sup> -doped crystal by PIXE/channeling technique: see	91Reb
Lattice site investigation for Mg in LiNbO <sub>3</sub> by combined RBS-PIXE-NRA channeling experiment: see	91Kli
Electron microscopic study of doped and proton-exchanged crystals: see	88Bur
Transmission electron microscope study of Ti-doped, congruent crystals: see	88Twi
Electron microscopic observation and electron diffraction study of proton-exchanged crystals: see	88Yan
<sup>181</sup> Hf → <sup>181</sup> Ta perturbed-angular correlation spectroscopy: Fig. 2A-1-137.	
PIXE, RBS and NRA yield profiles: Fig. 2A-1-138.	
Thermally stimulated charge emission and thermally stimulated light emission: Fig. 2A-1-139.	
Emission of electrons by illumination by light: see	88Roz
Plastic deformation of single crystals: see	87Fri
Efficiency of bulk acoustic wave convolvers (a review paper): see	89Cho5
Efficiency of transverse horizontal SAW convolvers usage (a review paper): see	89Cho6
Efficiency of transverse vertical SAW convolvers (a review paper): see	89Cho7
A review of signal processing using SAWs on LiNbO <sub>3</sub> : see	89Lew3
Miniaturized chip resonator: see	86Fuj
Electric field sensor using LiNbO <sub>3</sub> optical modulator: see	91Taj

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**Table 2A-1-001.** LiNbO<sub>3</sub> (undoped and Mg-, Ti-doped). Ferroelectric transition temperatures, birefringence and electrooptic constants [83Hol].

Crystal	$\Theta_{\text{f}}$ [°C]	$n_{\text{o}} - n_{\text{e}}$		$r_{13}$ [ $\cdot 10^{-12}$ mV $^{-1}$ ]		$r_{33}$ [ $\cdot 10^{-12}$ mV $^{-1}$ ]		
		$\lambda$ [ $\mu\text{m}$ ]	0.6328	1.32	0.6328	1.32	0.6328	1.32
undoped (congruent)	1130(2)		0.0837	0.0622	11.0(5)	10.3(10)	36.7(5)	34.1(10)
Mg-doped (10 mol%)	1160(2)		0.0861	0.0691	11.2(5)	9.7(10)	36.0(5)	34.0(10)
Ti-doped (3 mol%)	1130(2)		0.0804	0.0635	10.7(5)	9.3(10)	36.6(5)	33.6(10)

**Table 2A-1-002.** LiNbO<sub>3</sub>. Fractional coordinates and temperature parameters of atoms in the unit cell [66Abr2].  $B$  is defined by Eq. (e) in Introduction.

Atom	$x$	$y$	$z$	$B [\text{\AA}^2]$
Nb	0	0	0	0.50(1)
O	0.0492(4)	0.3446(5)	0.0647(4)	0.43(2)
Li	0	0	0.2829(23)	0.94(32)

**Table 2A-1-003.** LiNbO<sub>3</sub>. Fractional coordinates and temperature parameters of atoms in the unit cell [66Abr1]. *B* is defined by Eq. (e) in Introduction.

<i>T</i>	[°C]	24	250	500	750	1000	1200
<i>B</i> (Nb)	[Å <sup>2</sup> ]	−0.78(15)	−0.74(14)	−0.19(10)	−0.10(24)	0.39(24)	0.77(36)
<i>z</i> (Li)		0.2677(112)	0.2752(68)	0.2758(37)	0.2803(63)	0.2798(38)	*)
<i>B</i> (Li)	[Å <sup>2</sup> ]	1.12(248)	0.14(192)	−0.46(106)	−2.10(212)	−4.51(121)	*)
<i>x</i> (O)		0.0437(69)	0.0398(67)	0.0518(46)	0.0415(113)	0.0549(123)	0.0634(201)
<i>y</i> (O)		0.3309(82)	0.3238(89)	0.3318(65)	0.3073(188)	0.3253(198)	0.3375(315)
<i>z</i> (O)		0.0636(12)	0.0656(15)	0.0665(10)	0.0683(24)	0.0677(23)	0.0702(57)
<i>B</i> (O)	[Å <sup>2</sup> ]	−1.07(56)	−0.59(54)	0.04(34)	0.28(79)	0.09(88)	1.26(119)

\*) Not determinable.

**Table 2A-1-004.** LiNbO<sub>3</sub>. Interatomic distances and angles at 24 °C [66Abr2].

Distance	[Å]	Distance	[Å]	Angle	[°]	Angle	[°]
Nb–Nb	3.765(0)	O–O	2.719(4)	O–Nb–O	80.1(2)	O–Li–O	74.8(9)
Li–Li	3.765(0)		2.801(1)		88.7(1)		81.0(3)
Nb–O	1.889(3)		2.840(1)		90.3(1)		89.8(4)
	2.112(4)		2.879(4)		99.3(2)		108.7(9)
			3.042(2)	Average	89.6	Average	88.6
Nb–Li	3.010(31)		3.362(4)				
	3.054(7)						
	3.381(15)	Li–O	2.068(11)				
	3.922(31)		2.238(23)				

**Table 2A-1-005.** LiNbO<sub>3</sub>. Refined parameters for the neutron powder diffraction for displacive model [94Boy]. *n*: occupancy. The temperature parameters  $\beta_{ij}$  are defined by Eq. (c) in Introduction. In addition to the usual weighted profile agreement indicator

$$R_{wp} = \left[ \sum w(y_{obs} - y_{calc})^2 / \sum w y_{obs}^2 \right]^{1/2} \text{ and the corresponding goodness-of-fit}$$

$GOF_{wp} = R_{wp}/R_{pexp} = [w(y_{obs} - y_{calc})^2/(m - p)]^{1/2}$  [*y* are the individual profile intensities, *w* their weights, *m* their number and *p* the total (=structural + instrumental) number of refinable parameters], the weighted *R* factor for the integrated intensities  $R_{wl} = [R_{wp} = [\sum W(I_{obs} - I_{calc})^2 / \sum W I_{obs}^2]^{1/2}]$  is given. This allows comparison with a statistically expected  $R_{lexp}$ :  $GOF_{wl} = R_{wl}/R_{lexp} = [\sum W(I_{obs} - I_{calc})^2 / (M - P)]^{1/2}$ , where *I* are the reflection intensities, *W* their weights, *M* the number of reflections and *P* the number of structural parameters only.

<i>T</i> [K]	300	1200	1350	1450	1480	1505
	R3c	R3c	R3c	R $\bar{3}$ c	R $\bar{3}$ c	R $\bar{3}$ c
<i>z</i> (Li)	0.3021(9)	0.2885(17)	0.2850(10)	1/4	1/4	1/4
<i>z</i> (Nb)	0.0192(3)	0.0127(3)	0.0090(7)	0	0	0
<i>x</i> (O)	0.0478(4)	0.0573(6)	0.0564(11)	0.0591(4)	0.0602(6)	0.0598(18)
<i>y</i> (O)	0.3428(7)	0.3361(10)	0.3299(19)	1/3	1/3	1/3
<i>n</i> (Li)	1.02(4)	0.85(3)	0.87(4)	0.92(4)	0.91(6)	1.03(21)
<i>n</i> (Nb)	1.02(1)	1.00(1)	1.02(1)	1.01(1)	1.03(2)	1.00(6)
$\beta_{11}$ (Li)	0.014(6)	0.040(5)	0.054(8)	0.043(7)	0.028(9)	0.053(33)
$\beta_{33}$ (Li)	0.006(2)	0.014(3)	0.002(2)	0.039(3)	0.033(5)	0.053(21)
$\beta_{11}$ (Nb)	0.003(2)	0.020(1)	0.021(1)	0.021(1)	0.021(2)	0.014(6)
$\beta_{33}$ (Nb)	0.0003(–) *)	0.0018(2)	0.0015(2)	0.0021(2)	0.0027(3)	0.0027(9)
$\beta_{11}$ (O)	0.001(2)	0.030(2)	0.034(5)	0.029(1)	0.030(2)	0.028(6)
$\beta_{22}$ (O)	0.002(1)	0.020(1)	0.021(1)	0.027(1)	0.023(2)	0.019(6)
$\beta_{33}$ (O)	0.0006(1)	0.0027(1)	0.0036(2)	0.0035(1)	0.0032(2)	0.0027(6)
$\beta_{12}$ (O)	–0.002(1)	0.012(2)	0.018(4)	0.013	0.012	0.009
$\beta_{13}$ (O)	0.0005(5)	–0.0035(7)	–0.0051(8)	–0.0023(1)	–0.0023(2)	–0.0018(6)
$\beta_{23}$ (O)	–0.0006(3)	–0.0034(2)	–0.0047(3)	–0.0046	–0.0047	–0.0035
<i>a</i> [Å]	5.1513(8)	5.2542(6)	5.2718(8)	5.2850(8)	5.2898(12)	5.2924(36)
<i>c</i> [Å]	13.8654(8)	13.8759(6)	13.8604(9)	13.8488(8)	13.8485(12)	13.8462(39)
<i>R</i> <sub>wp</sub> [%]	9.62	6.81	9.37	8.60	12.98	13.17
<i>GOF</i> <sub>wp</sub>	2.74	2.04	1.33	1.97	1.59	2.69
<i>R</i> <sub>wl</sub> [%]	4.87	1.68	4.74	4.46	8.63	9.23
<i>GOF</i> <sub>wl</sub>	6.40	2.34	2.98	4.17	4.25	7.49

\*) At room temperature Nb was refined isotropically to avoid (non-significant) negative  $\beta_{33}$ .

**Table 2A-1-006.** LiNbO<sub>3</sub>. Refined parameters for the neutron powder diffraction for disorder model [94Boy]. See also the caption of Table 2A-1-005.

$T$ [K]	1200	1350	1450	1480	1505
	R3c	R3c	R $\bar{3}c$	R $\bar{3}c$	R $\bar{3}c$
$z(\text{Li})$	0.2875(17)	0.2762(13)	0.2813(8)	0.2812(10)	0.2905(39)
$z(\text{Nb})$	0.0128(4)	0.0093(7)	0	0	0
$x(\text{O})$	0.0576(6)	0.0569(9)	0.0595(3)	0.0607(5)	0.0597(15)
$y(\text{O})$	0.3369(11)	0.3297(15)	1/3	1/3	1/3
$n(\text{Li})/n(\text{Li}')$	0.75(8)/0.10(8)	0.33(7)/0.57(8)	0.85(3)	0.85(5)	1.00(18)
$n(\text{Nb})$	1.00(1)	0.99(1)	1.01(1)	1.04(2)	0.99(6)
$\beta_{11}(\text{Li})$	0.040(5)	0.070(9)	0.047(6)	0.030(8)	0.059(33)
$\beta_{33}(\text{Li})$	0.012(4)	0.002(1)	0.001(1)	0.002(2)	0.003(6)
$\beta_{11}(\text{Nb})$	0.020(1)	0.018(1)	0.021(1)	0.020(2)	0.013(6)
$\beta_{33}(\text{Nb})$	0.0018(2)	0.0019(2)	0.0017(2)	0.0023(3)	0.0026(9)
$\beta_{11}(\text{O})$	0.028(2)	0.036(5)	0.028(1)	0.028(2)	0.029(6)
$\beta_{22}(\text{O})$	0.0200(9)	0.022(1)	0.026(1)	0.022(2)	0.019(6)
$\beta_{33}(\text{O})$	0.0027(1)	0.0034(2)	0.0034(1)	0.0029(2)	0.0024(6)
$\beta_{12}(\text{O})$	0.011(2)	0.018(4)	0.013	0.011	0.010
$\beta_{13}(\text{O})$	−0.0030(8)	−0.0020(10)	−0.0023(1)	−0.0024(2)	−0.0019(6)
$\beta_{23}(\text{O})$	−0.0034(2)	−0.0047(3)	−0.0047	−0.0047	−0.0037
$a$ [Å]	5.2542(6)	5.2719(8)	5.2849(8)	5.2897(12)	5.2923(36)
$c$ [Å]	13.8759(6)	13.8601(8)	13.8481(8)	13.8476(12)	13.8451(36)
$R_{\text{wp}}$ [%]	6.81	9.05	8.51	12.66	12.62
$\text{GOF}_{\text{wp}}$	2.04	1.29	1.95	1.55	2.58
$R_{\text{wl}}$ [%]	1.68	4.20	4.25	7.74	8.61
$\text{GOF}_{\text{wl}}$	2.38	2.69	4.03	3.87	7.10



**Table 2A-1-007.** LiNbO<sub>3</sub>. Elastic, piezoelectric, dielectric constants and their temperature coefficients. For definition of temperature coefficients, see original paper.  $\kappa$  at  $f = 500$  Hz. [71Smi, 67War, 67Yam].

	Absolute quantities			Normalized temperature coeff.	
	[71Smi]	[67War]	[67Yam]	[71Smi]	[67Yam]
Elastic stiffnesses	[ $\cdot 10^{11}$ Nm <sup>-2</sup> ]	[ $\cdot 10^{11}$ Nm <sup>-2</sup> ]		[ $\cdot 10^{-4}$ K <sup>-1</sup> ]	[ $\cdot 10^{-4}$ K <sup>-1</sup> ]
$c_{11}^E$	2.030	2.03		-1.74	
$c_{12}^E$	0.573	0.53		-2.52	
$c_{13}^E$	0.752	0.75		-1.59	
$c_{14}^E$	0.085	0.09		-2.14	
$c_{33}^E$	2.424	2.45		-1.53	
$c_{44}^E$	0.595	0.60		-2.04	
$c_{66}^E$	0.728	0.75		-1.43	
Elastic compliances	[ $\cdot 10^{-12}$ m <sup>2</sup> N <sup>-1</sup> ]	[ $\cdot 10^{-12}$ m <sup>2</sup> N <sup>-1</sup> ]	[ $\cdot 10^{-12}$ m <sup>2</sup> N <sup>-1</sup> ]		
$s_{11}^E$	5.831	5.78	5.64	1.66	1.5
$s_{12}^E$	-1.150	-1.01		0.28	
$s_{13}^E$	-1.452	-1.47		1.94	
$s_{14}^E$	-1.000	-1.02	-0.84	1.33	
$s_{33}^E$	5.026	5.02	4.94	1.60	1.5
$s_{44}^E$	17.10	17.0		2.05	
$s_{66}^E$	13.96	13.6		1.43	
Piezoelectric stress constants	[Cm <sup>-2</sup> ]	[Cm <sup>-2</sup> ]			
$e_{15}$	3.76	3.7		1.47	
$e_{22}$	2.43	2.5		0.79	
$e_{31}$	0.23	0.2		2.21	
$e_{33}$	1.33	1.3		8.87	
Piezoelectric strain constants	[ $\cdot 10^{-11}$ CN <sup>-1</sup> ]	[ $\cdot 10^{-11}$ CN <sup>-1</sup> ]	[ $\cdot 10^{-11}$ CN <sup>-1</sup> ]		
$d_{15}$	6.92	6.8	7.4	3.45	2.8
$d_{22}$	2.08	2.1	2.1	2.34	2.4
$d_{31}$	-0.085	-0.1	-0.087	19.1	11.0
$d_{33}$	0.60	0.6	1.6	11.3	2.9
Dielectric constants					
$\kappa_{11}^S$	44.3	44		3.23	
$\kappa_{33}^S$	27.9	29		6.27	
$\kappa_{11}^T$	85.2	84	84.6	3.82	
$\kappa_{33}^T$	28.7	30	28.6	6.71	

**Table 2A-1-008.** LiNbO<sub>3</sub>. Third-order dielectric constants [in 10<sup>-19</sup> C V<sup>-2</sup>] [87Cho].

$\kappa_{311}$	-2.81(6)
$\kappa_{222}$	-2.40(9)
$\kappa_{333}$	-2.91(6)

**Table 2A-1-009.** LiNbO<sub>3</sub>. Nonlinear piezoelectric constants [in C m<sup>-2</sup>] [75Kor].

$e_{115}$	-58	$e_{311}$	4
$e_{116}$	-26	$e_{312}$	-6
$e_{125}$	12	$e_{313}$	15
$e_{126}$	-4	$e_{314}$	-23
$e_{135}$	53	$e_{333}$	-10
$e_{136}$	185	$e_{344}$	-3
$e_{145}$	17		

**Table 2A-1-010.** LiNbO<sub>3</sub>. Electrostrictive constants [in 10<sup>-9</sup> N V<sup>-2</sup>] [87Cho].  $R_{\lambda\mu}=R_{\text{klij}}$ .  $R_{\text{klij}}$  is defined by the equation  $T_{ij} = -(1/2)R_{\text{klij}}E_kE_l$ , where  $T_{ij}$  is a stress component and  $E_k$  is an electric field.

$R_{11}$	1.11(39)	$R_{33}$	-2.76(41)
$R_{12}$	2.19(56)	$R_{14}$	1.51(17)
$R_{13}$	2.32(67)	$R_{41}$	1.85(17)
$R_{31}$	0.19(61)	$R_{44}$	-1.83(11)

**Table 2A-1-011.** LiNbO<sub>3</sub>. Third-order piezoelectric constants [in C m<sup>-2</sup>] [87Cho].

$e_{222}$	15.0	$e_{311}$	14.7
$e_{115}$	17.1	$e_{312}$	13.0
$e_{125}$	19.9	$e_{313}$	-10.0
$e_{126}$	-15.9	$e_{314}$	11.0
$e_{135}$	19.6	$e_{333}$	-17.3
$e_{136}$	-0.9	$e_{344}$	-10.2
$e_{145}$	20.3		

**Table 2A-1-012.** LiNbO<sub>3</sub>, LiTaO<sub>3</sub>. Values of the sound velocity and attenuation of various modes measured by the acoustooptic method [84Bli]. L: longitudinal mode, S: shear mode. Q denotes the quasi-mode.  $f \cong 1\text{GHz}$ .

Propagation direction	Type of wave	LiNbO <sub>3</sub>		LiTaO <sub>3</sub>	
		$\nu$ [km s <sup>-1</sup> ]	$\alpha$ [·10 <sup>2</sup> m <sup>-1</sup> ]	$\nu$ [km s <sup>-1</sup> ]	$\alpha$ [·10 <sup>2</sup> m <sup>-1</sup> ]
[100]	L	6.589	0.115	5.580	0.139
	S <sub>1</sub>	4.730	0.088	4.252	0.128
	S <sub>2</sub>	4.071	0.113	3.351	0.187
[010]	QL	6.863	0.101	5.802	0.123
	S	3.944	0.123	3.545	0.168
[001]	L	7.345	0.055	6.179	0.068
	S	3.627	0.206	3.602	0.200
[011]	QL	7.375	0.065	6.210	0.092
	S	4.064	0.107	3.400	0.248
[101]	QL	7.313	0.067	6.012	0.065
	QS <sub>1</sub>	4.054	0.096	—	—
[110]	QL	6.691	0.080	5.682	0.111
	QS <sub>1</sub>	4.003	0.106	3.581	0.120

**Table 2A-1-013.** LiNbO<sub>3</sub>. Summary of design data for microwave acoustic surface wave devices [73Sza]. prop: propagation, Vac attn: (surface wave) attenuation in vacuum, Sw: surface wave, bw: bandwidth. See also [72Sch].

Orientation	Y cut Z prop	16 ½° double rotated cut	41 ½° rotated cut X prop	Z cut X prop	X cut Z prop
Surface wave velocity $v_{\infty}$ [m s <sup>-1</sup> ]	3488	3503	4000	3798	3483
Estimate of electromagnetic to acoustic coupling $\Delta v/v_{\infty}$	0.0241	0.0268	0.0277	0.0026	0.0252
Measured value of $\Delta v/v_{\infty}$ <sup>a)</sup>	0.0214	0.0227	0.0273		
Power flow angle $\phi$ [°] (electromechanical)	0	0	0	0	-1.726
Temperature coefficient of delay ( $1/\tau$ ) $\partial\tau/\partial T$ [ $\cdot 10^{-6}$ K <sup>-1</sup> ]	94	96	72	77	93
Sw attn in air at 1 GHz [dB/μs]	1.07	1.15	1.05	0.93	—
Air loading at 1 GHz [dB/μs]	0.19	0.21	0.3	0.24	—
Vac attn at 1 GHz [dB/μs]	0.88	0.94	0.75	0.69	—
3 dB Air prop loss time delay at 1 GHz $A$ [μs]	2.8	2.6	2.9	3.2	—
Slope of electromechanical power flow curve $\partial\phi/\partial\theta$ <sup>b)</sup>	-1.083	-1.087	-0.445	+0.192	-0.610
Slope of electromechanical power flow curve $\partial\phi/\partial\mu$ <sup>c)</sup>	-0.117	+0.151	0	0	0
3 dB Beam steering loss time delay $B$ [μs]	7.4	7.0	18.9	46.0	15.8
3 dB Diffraction loss time delay at 1 GHz $C$ [μs]	29.1	29.3	5.1	2.4	7.6
Material figure of merit $F_M = ABC \left( \frac{\Delta v}{v_{\infty}} \right)^2$	0.350	0.383	0.214	0.002	—
Time-bw product figure of merit $F_{TB} = \frac{4 \cdot 10^3 ABC}{v_{\infty}} \left( \frac{\Delta v}{v_{\infty}} \right)^2$	0.402	0.437	0.214	0.003	—

<sup>a)</sup> [72Sch]. <sup>b)</sup>  $\theta$ : direction of propagation. <sup>c)</sup>  $\mu$ : direction of plate normal.

**Table 2A-1-014.** LiNbO<sub>3</sub>. Third-order elastic constants [in 10<sup>11</sup> N m<sup>-2</sup>] at 20 °C [73Nak].

$c_{111}^E$	-5.12(194)	$c_{134}^E$	-0.01(26)
$c_{112}^E$	4.54(76)	$c_{144}^E$	-0.37(20)
$c_{113}^E$	7.28(172)	$c_{155}^E$	-5.99(26)
$c_{114}^E$	-4.10(44)	$c_{222}^E$	-4.78(187)
$c_{123}^E$	7.19(147)	$c_{333}^E$	-3.63(690)
$c_{124}^E$	0.55(13)	$c_{344}^E$	-5.40(29)
$c_{133}^E$	-0.34(173)	$c_{444}^E$	-0.41(92)



**Table 2A-1-015.** LiNbO<sub>3</sub>. Third-order elastic constants [in 10<sup>11</sup> N m<sup>-2</sup>] [87Cho].

$c_{111}$	-21.2	$c_{134}$	1.5
$c_{112}$	-5.3	$c_{144}$	-3.0
$c_{113}$	-5.7	$c_{155}$	-6.7
$c_{114}$	2.0	$c_{222}$	-23.3
$c_{123}$	-2.5	$c_{333}$	-29.6
$c_{124}$	0.4	$c_{344}$	-6.8
$c_{133}$	- 7.8	$c_{444}$	-0.3

**Table 2A-1-016.** LiNbO<sub>3</sub>. Refractive indices of congruent LiNbO<sub>3</sub> at 24.5 °C [74Nel]. See also [67Boy, 68Mid, 76Smi].

$\lambda$ [μm]	$n_o$	$n_e$	$\lambda$ [μm]	$n_o$	$n_e$
0.40463	2.4317	2.3260	0.95998	2.2393	2.1622
0.43584	2.3928	2.2932	1.0140	2.2351	2.1584
0.46782	2.3634	2.2683	1.09214	2.2304	2.1545
0.47999	2.3541	2.2605	1.15392	2.2271	2.1517
0.50858	2.3356	2.2448	1.15794	2.2269	2.1515
0.54607	2.3165	2.2285	1.28770	2.2211	2.1464
0.57696	2.3040	2.2178	1.43997	2.2151	2.1413
0.57897	2.3032	2.2171	1.63821	2.2083	2.1356
0.58756	2.3002	2.2147	1.91125	2.1994	2.1280
0.64385	2.2835	2.2002	2.18428	2.1912	2.1211
0.66782	2.2778	2.1953	2.39995	2.1840	2.1151
0.70652	2.2699	2.1886	2.61504	2.1765	2.1087
0.80926	2.2541	2.1749	2.73035	2.1724	2.1053
0.87168	2.2471	2.1688	2.89733	2.1657	2.0999
0.93564	2.2412	2.1639	3.05148	2.1594	2.0946

**Table 2A-1-017.** LiNbO<sub>3</sub>:MgO. Principal refractive indices of the crystal doped with 5 mol% MgO [92She].

$\lambda$ [ $\mu\text{m}$ ]	$n$	20.0 °C	74.5 °C	116.0 °C	154.5 °C
0.53975	$n_o$	2.3120	2.3129	2.3137	2.3142
	$n_e$	2.2194	2.2230	2.2261	2.2292
0.6328	$n_o$	2.2792	2.2798	2.2804	2.2808
	$n_e$	2.1916	2.1950	2.1978	2.2003
1.0795	$n_o$	2.2251	2.2254	2.2256	2.2257
	$n_e$	2.1454	2.1481	2.1504	2.1527
1.3414	$n_o$	2.2126	2.2130	2.2132	2.2134
	$n_e$	2.1349	2.1376	2.1398	2.1420

**Table 2A-1-018.** LiNbO<sub>3</sub>. Refractive indices at various wavelengths [90Jun]. Sample: almost stoichiometric (Li/Nb  $\cong$  1.00) crystal prepared by vapor transport equilibrium.

$\lambda$ [nm]	$n_e$	$n_o$
1064	2.1440(5)	2.2339(5)
632.8	2.1890(4)	2.2878(5)
514.5	2.2270(4)	2.3334(4)
501.7	2.2329(4)	2.3405(4)
496.5	2.2352(5)	2.3437(4)
488.0	2.2398(4)	2.3495(4)
476.5	2.2465(4)	2.3573(5)
472.7	2.2489(5)	2.3604(5)
465.8	2.2530(4)	2.3658(4)
457.9	2.2584(4)	2.3719(4)
454.5	2.2608(4)	2.3751(5)
325.0	2.4670(5)	2.6360(20)

**Table 2A-1-019.** LiNbO<sub>3</sub>. Refractive indices at RT with the addition of transition metals [79Sir].

Impurity ion	[at%]	$n_o$						
		$\lambda$ [μm]	0.4047	0.4713	0.4800	0.5461	0.5852	0.5876
Pure	—		2.3925	2.3456	2.3431	2.3164	2.3040	2.3033
Sc	0.1		2.3935	2.3466	2.3436	2.3172	2.3100	2.3040
Ti	0.1		2.3928	2.3462	2.3432	2.3167	2.3043	2.3036
Cr	0.1		2.3926	—	—	2.3167	2.3042	2.3035
Mn	0.1		2.3944	—	—	2.3180	2.3056	2.3047
Fe	0.1		2.3930	2.3464	2.3434	2.3166	2.3044	2.3036
Co	0.1		2.3942	—	—	2.3176	2.3052	2.3046
Ni	0.1		2.3933	2.3466	2.3437	2.3170	2.3046	2.3038
Cu	0.5		—	—	—	2.3176	2.3051	2.3043
Zn	0.2		2.3929	—	—	2.3171	2.3046	2.3038

  

Impurity ion	[at%]	$n_e$						
		$\lambda$ [μm]	0.4047	0.4713	0.4800	0.5461	0.5852	0.5876
Pure	—		2.2874	2.2484	2.2461	2.2237	2.2130	2.2124
Sc	0.1		2.2883	2.2495	2.2471	2.2249	2.2143	2.2137
Ti	0.1		2.2881	2.2491	2.2468	2.2241	2.2136	2.2129
Cr	0.1		2.2852	—	—	2.2217	2.2112	2.2105
Mn	0.1		2.2868	—	—	2.2232	2.2128	2.2119
Fe	0.1		2.2878	2.2487	2.2464	2.2234	2.2135	2.2128
Co	0.1		2.2899	—	—	2.2262	2.2154	2.2147
Ni	0.1		2.2879	2.2488	2.2468	2.2240	2.2136	2.2129
Cu	0.5		—	—	—	2.2247	2.2141	2.2134
Zn	0.2		—	—	—	2.2243	2.2137	2.2131

**Table 2A-1-020.** LiNbO<sub>3</sub>. Electrooptic constants, [67Zoo]. See also [66Ber, 67Sma, 72Onu, 66Tur1, 66Tur2].

	$r_{13}$	$r_{33}$	$r_{51}$	$r_{22}$	$r_c$	$\lambda$	Ref.
	[ $\cdot 10^{-12} \text{ mV}^{-1}$ ]					[ $\mu\text{m}$ ]	
$r^{\text{T}}$	10	32.2	32	6.8		0.633	67Zoo
				3.2	17.4	0.633	66Ber
				6.7	18	0.633	67Sma
				5.7	17	1.15	
				3.1	16	3.39	
						0.633	72Onu
$r^{\text{S}}$	10.9	34.0					
	8.6	30.8	28	3.4		0.633	66Tur1
	6.5	28	23	3.1		3.39	66Tur2

**Table 2A-1-021.** LiNbO<sub>3</sub>. Piezooptic constants  $p_{\lambda\mu}^E$  [76Ava2]. See also [67Dix, 71Lem, 70OBr, 73Mar, 71Klu].

$p_{11}$	$p_{33}$	$p_{44}$	$p_{66}$	$p_{12}$	$p_{13}$	$p_{14}$	$p_{31}$	$p_{41}$	Ref.
0.036	0.066	—	—	0.072	0.135	—	0.178	0.155	67Dix
0.025	0.068	—	—	0.079	0.132	0.100	0.168	0.158	71Lem
0.034	0.060	0.300	—	0.072	0.139	0.066	0.178	0.154	70OBr
—	0.069	0.152	0.055	0.088	0.126	0.080	0.176	0.134	73Mar
0.021 (0.045)	0.078	0.019	—	0.096	0.149	0.055	0.138	—	71Klu
−0.026	+0.071	+0.146	−0.053	+0.090	+0.133	−0.075	+0.179	−0.151	76Ava2

**Table 2A-1-022.** LiNbO<sub>3</sub>. Piezooptical coefficients [91Myt]. For definitions of  $\Pi_{im}^0$ ,  $\Pi_{km}^0$  and  $\delta\Delta_k$ , see original paper.

Experimental $\Pi_{im}$ conditions	contribution into $\delta\Delta_k$ [%]		calculated $\Pi_{km}^*$	$\Pi_{km}^*$ derived from $\Pi_{km}^0$			Other data for $\Pi_{km}^0$	
	$\Pi_{im}$	$s_{km}$		$\Pi_{km}^0$	Elasticity contribut.	$\Pi_{km}^*$	[66Spe]	[79Vas]
m = 1 i = 1 $\Pi_{11} = -0.45$	227	-127	$\Pi_{21}^* = \Pi_{31}n_3^3 -$	+10.2	+0.20	+10.4	–	16.8
k = 2 i = 3 $\Pi_{31} = +0.49$	65	35	$\Pi_{11}n_1^3 = +10.6$					
m = 1 i = 1 $\Pi_{11} = -0.48$	238	-138	$\Pi_{31}^* = \Pi_{11}n_1^3 -$	-6.9	0	-6.9	12.2	15.1
k = 3 i = 2 $\Pi_{21} = +0.11$	28	72	$\Pi_{21}n_2^3 = -7.0$					
m = 2 i = 2 $\Pi_{22} = -0.46$	227	-127	$\Pi_{12}^* = \Pi_{22}n_2^3 -$	-10.5	-0.20	-10.7	7.33	7.36
k = 1 i = 3 $\Pi_{32} = +0.45$	63	37	$\Pi_{32}n_3^3 = -10.3$					
m = 2 i = 1 $\Pi_{12} = +0.11$	28	72	$\Pi_{32}^* = \Pi_{12}n_1^3 -$	+6.7	0	+6.7	8.25	8.94
k = 3 i = 2 $\Pi_{22} = -0.49$	238	-138	$\Pi_{22}n_2^3 = +7.0$					
m = 3 i = 2 $\Pi_{23} = +2.0$	88	12	$\Pi_{13}^* = \Pi_{23}n_2^3 -$	+6.2	-0.22	+6.0	5.16	17.4
k = 1 i = 3 $\Pi_{33} = +1.7$	85	15	$\Pi_{33}n_3^3 = +5.7$					
m = 3 i = 1 $\Pi_{13} = +0.9$	87	13	$\Pi_{23}^* = \Pi_{33}n_3^3 -$	-5.3	+0.22	-5.1	8.62	15.9
k = 2 i = 3 $\Pi_{33} = +1.5$	83	17	$\Pi_{13}n_1^3 = -5.9$					
m = 4 i = 1 $\Pi_{14} = +0.7$	m = 1 i = 4		m = 4 i = 4					
k = $\bar{4}$	k = $\bar{4}$ $\Pi_{41} = -1.9$		k = $\bar{4}$ $\Pi_{44} = +0.23$					



**Table 2A-1-023.** LiNbO<sub>3</sub>. Assignment of optical phonon modes [72Cla]. Frequencies are given in cm<sup>-1</sup>. The result of [72Cla] is from Raman scattering and the accuracy is  $\pm 2$  cm<sup>-1</sup>. The results of [67Kam] and [66Sch] are from Raman, while the results of [67Bar] is from Raman and infrared experiments. Main differences between [72Cla] and others are indicated by arrows at the right-hand side of the table. Modes indicated by an asterisk are assumed to be of second order.

[72Cla]		[67Kam]		[67Bar]		[66Sch]		
	Raman		Raman		Raman	IR	Raman	
		E(T)	92					←
		E(L)	117:95					←
E(T)	155	E(T)	152	E(T)	152	152	E(T)	152
E(L)	198	E(L)	198	E(L)		198		
E(T)	238	E(T)	238	E(T)	238	236	E(T)	239
E(L)	243	E(L)	243	E(L)		238		
A <sub>1</sub> (T)	255	A <sub>1</sub> (T)	253	A <sub>1</sub> (T)	252	248	A <sub>1</sub> (T)	255
E(T)	265	E(T)	262	E(T)	264	265	E(T)	266
A <sub>1</sub> (L)	275	A <sub>1</sub> (L)	273	A <sub>1</sub> (L)		273		
A <sub>1</sub> (T)	276	A <sub>1</sub> (T)	275	A <sub>1</sub> (T)	276	274	A <sub>1</sub> (T)	277
E(L)	295	E(L)	298	E(L)	299	296		
E(T)	325	E(T)	322	A <sub>1</sub> (L)		306	E(T)	321
A <sub>1</sub> (L)	333	A <sub>1</sub> (L)	331	E(T)	321	322		←
A <sub>1</sub> (T)	334	A <sub>1</sub> (T)	334	A <sub>1</sub> (T)	333	307		
E(L)	371	E(L)	345	E(L)	333	342		
E(T)	371	E(T)	368	E(T)	367	363	E(T)	369
E(L)	428	E(L)	428	E(L)		418		
E(T)	431	A <sub>1</sub> (L)	428	A <sub>1</sub> (L)		423	E(T)	430
A <sub>1</sub> (L)	436	E(T)	436	E(T)	434	431		←
E(L)	454	E(L)	448	E(L)		450		
E(T)	582	E(T)	582	E(T)	579	586	E(T)	580
A <sub>1</sub> (T)	633	E(L)	621	A <sub>1</sub> (T)	634	628	A <sub>1</sub> (T)	632
E(L)	668	E(T)	630	*E(L)		660		←
E(T)	668	A <sub>1</sub> (T)	637	*E(T)		670		←
E(L)	739			*A <sub>1</sub> (L)		686		←
E(T)	743			*A <sub>1</sub> (T)		692		←
A <sub>1</sub> (L)	876	A <sub>1</sub> (L)	874	A <sub>1</sub> (L)	873	869		
E(L)	880	E(L)	881	E(L)	880	878	E(L)	883

**Table 2A-1-024.** LiNbO<sub>3</sub>. Brillouin scattering [71Kha]. Geometry [for example  $z(xz)y$ ] from left to right: propagation direction of the incident light, polarization of the incident light, polarization of the scattered light and propagation direction of the scattered light. Direction: phonon propagation direction,  $\Delta\nu$ : phonon frequency, \*: intense lines,  $v_{\text{exp}}$ : experimental phonon velocity,  $v_{\text{calc}}$ : calculated phonon velocity, P: phonon polarization, ql: quasi-longitudinal, qt: quasi-transverse, t: transverse.

Geometry	Direction	$\Delta\nu/c$ [ $\cdot 10^2 \text{ m}^{-1}$ ]	$v_{\text{exp}}$ [ $\cdot 10^3 \text{ m s}^{-1}$ ]	$v_{\text{calc}}$ [ $\cdot 10^3 \text{ m s}^{-1}$ ]	P
$y(xy)x$	$k_x = \sqrt{2}/2$	0.92	5.67	5.65	ql
$y(zz)x$	$k_y = -\sqrt{2}/2$	0.94	5.79	5.65	ql
$y(xz)x$	$k_z = 0$ $k_x = 0$	0.56*	3.45	3.40	qt
$z(xz)y$	$k_y = \sqrt{2}/2$	0.63*	3.88	3.75	t
$z(xx)y$	$k_z = -\sqrt{2}/2$	1.02*	6.29	5.94	ql
$\bar{z}(xx)y$	$k_x = 0$	1.00	6.16	6.31	ql
$\bar{z}(xz)y$	$k_y = \sqrt{2}/2$	0.56*	3.45	3.32	t
$\bar{z}(yx)y$	$k_z = \sqrt{2}/2$	0.56	3.45	3.32	t
$z(yx)x$	$k_x = \sqrt{2}/2$	0.58*	3.57	3.59	qt
$z(yy)x,$ $z(xz)x$	$k_y = 0$	1.07*	6.59	6.17	ql
$z(xy)x$	$k_z = -\sqrt{2}/2$	$\begin{cases} 1.06 \\ 0.56 \\ 0.56 \end{cases}$	$\begin{cases} 6.53 \\ 3.45 \\ 3.45 \end{cases}$	$\begin{cases} 6.17 \\ 3.37 \\ 3.37 \end{cases}$	$\begin{cases} \text{ql} \\ \text{qt} \\ \text{qt} \end{cases}$

**Table 2A-1-025.** LiNbO<sub>3</sub>. <sup>93</sup>Nb NMR [70Sch].  $\nu_i$ : transition frequencies.  
 $\nu_1: \pm 3/2 \leftrightarrow \pm 1/2$ ,  $\nu_2: \pm 5/2 \leftrightarrow \pm 3/2$ ,  $\nu_3: \pm 7/2 \leftrightarrow \pm 5/2$ ,  $\nu_4: \pm 9/2 \leftrightarrow \pm 7/2$ .

$T$	77 K	24...25 °C	167 °C
$\nu_1$ [MHz]	0.988	0.924	–
$\nu_2$ [MHz]	1.958	1.842	1.725
$\nu_3$ [MHz]	2.942	2.763	2.589
$\nu_4$ [MHz]	3.950	3.685	–
$e^2qQ/h$ [MHz]	23.516	22.10	20.70
$\eta$	<3%	<3%	<1%

**Table 2A-1-026.** LiNbO<sub>3</sub>. ESR data [70Rex, 72Her, 68Dan]. See also [72McD, 68Bur, 67Evl].

Paramagnetic center		Cr <sup>3+</sup>		Fe <sup>3+</sup>	Mn <sup>2+</sup>	Mn <sup>2+</sup>
Site		Nb <sup>5+</sup>	Li <sup>1+</sup>	Nb <sup>5+</sup> or Li <sup>1+</sup>	Nb <sup>5+</sup> or Li <sup>1+</sup>	
$S$		3/2		5/2	5/2	5/2
$\nu$	[GHz]	9		9.4 and 35.4	9.4 and 35.4	X-band and K-band
$T$	[K]	77		300	300	RT
$g$ -factors		1.969	1.97	2.0024	2.0002	$g_{\parallel} = g_{\perp} = 1.990$
FS	[ $\cdot 10^{-2} \text{ m}^{-1}$ ]	$D = 4110$	$D = 2100$ (200)	$2D = 3319$ $a-F = 128$	$2D = 1449$ $a-F = 8$	$b_{20} = 726$ $b_{40} = -2$
HFS	[ $\cdot 10^{-2} \text{ m}^{-1}$ ]				79	$A_{\parallel} = -78.2$ $A_{\perp} = -76.7$
Ref.		70Rex		72Her	68Dan	68Dan

**Table 2A-1-027.** LiNbO<sub>3</sub>:Gd<sup>3+</sup>.  $g$  values and crystal field parameters [73Dis]. Crystal field parameters are given in units of m<sup>-1</sup>.

Parameter	LiNbO <sub>3</sub> :Gd <sup>3+</sup> Pattern I	LiNbO <sub>3</sub> :Gd <sup>3+</sup> Pattern II
$g_{\parallel} = g_z$	1.9916(5)	1.9916(5)
$g_{\perp} = g_x = g_y$	1.9916(10)	1.9916(10)
$b_{20}$	+1185(13)	+1260(20)
$b_{40}$	+ 8(3)	+ 8(4)
$b_{60}$	+ 1(1)	+ 1(2)
$ b_{43} $	33(17)	33(17)
$b_{22}$	0(5)	+ 40(10)

**Table 2A-1-028.** LiNbO<sub>3</sub>. Spin Hamiltonian parameters for Cu<sup>2+</sup> ESR [84Pet].  
 $g'_{\parallel}$ ,  $g'_{\perp}$  : averaged  $g$ -tensor components parallel and perpendicular to the polar axis, respectively.

Principal values of $g$ -tensor	Principal values of $A$ -tensor [ $\cdot 10^{-2} \text{ m}^{-1}$ ]
$g_z = 2.403(5)$	$A_z = 82(2)$
$g_y = 2.121(7)$	$A_y = 29(3)$
$g_x = 2.095(5)$	$A_x = 40(2)$
$g'_{\parallel} = 2.22(2)$	
$g'_{\perp} = 2.17(2)$	

**Table 2A-1-029.** LiNbO<sub>3</sub>:Cr<sup>3+</sup>. Spin Hamiltonian parameters and the proposed assignment of Cr<sup>3+</sup> sites [93Yeo].

Spectra	$g$	$D$ [ $\cdot 10^2 \text{ m}^{-1}$ ]	Site	Methods	Ref.
Main signal	1.97	0.45	Nb	EPR	67Evl
			Nb	Optical spectra	69Gla, 73Cla
	$g_{\parallel} = 1.969$	0.45		Optical spectra, EPR	69Bur
	$g_{\perp} = 3.870$				
	1.969	0.411	Nb	EPR	70Rex
	1.97	0.21	Li		
			Li and Nb	Flourescence spectra	90Jia
			Nb	Optical spectra	82Kim
	1.969	0.396	Li	EPR	83Mal
	1.969	0.396	Li or Nb	EPR	85Mal, 85Gra
			Li, Nb, SV	EPR	86Mal
	1.97	0.393		EPR	87Gra, 89Cho, 91Yeo
	1.97	-0.392		EPR and ENDOR	87Gra
	1.972	0.395	Li	EPR and NMR	86Cho, 89Cho, 91Yeo
			Li and Nb	EPR and ENDOR	89Gli
Cr <sup>3+</sup> (main)	1.96	0.39		EPR	91Siu
	1.968	0.393		EPR	93Par1
Cr <sup>3+</sup> (weak)	1.968	0.443			
Cr <sub>I</sub> <sup>3+</sup> (main)	1.957	0.393	Li	EPR	93Yeo
Cr <sub>II</sub> <sup>3+</sup> (weak)	1.96	0.1	Nb		

**Table 2A-1-030.** LiNbO<sub>3</sub>. ESR parameters for Nb<sup>4+</sup> [92Mul].  $\theta_g$ ,  $\theta_A$ : tilt angles of principal axes of  $g$ - and  $A$ -tensors from the  $c$ -axis.

$g'_x$	$\approx 1.709$	$A_x$	$\approx 584$	MHz
$g'_y$	$\approx 1.795$	$A_y$	$\approx 677$	MHz
$g'_z$	$\approx 1.883$	$A_z$	$\approx 258$	MHz
$\theta_g$	$\approx -11^\circ$	$\theta_A$	$\approx -15^\circ$	



**Table 2A-1-031.** LiNbO<sub>3</sub>:Fe<sup>3+</sup>. Spin-Hamiltonian parameters and the proposed site assignments for Fe<sup>3+</sup> [94Yeo1].

$g$	FS [ $\cdot 10^{-2} \text{ m}^{-1}$ ]	Site	Method	Ref.
1.99	$b_2^0 = 1671(28), b_4^0 = -48(11), b_4^3 = 560(280)$	mostly Nb <sup>5+</sup> <sup>b)</sup>	EPR*	79Tow
$g_{\parallel} = 2.0024(5)$	$b_2^0 = 1660(3), b_4^0 = -43(2), b_4^3 = -1537(235)$	Li <sup>+</sup> or Nb <sup>5+</sup>	EPR*	72Her
1.995(5)	$b_2^0 = 1530,  b_4^0  = 714$		EPR	72Meh2
1.993	$b_2^0 = 1650, b_4^0 = -118.8, b_4^3 = 1360.8$	Li <sup>+</sup> , Nb <sup>5+</sup> , V	EPR*	85Cho
1.993	$b_2^0 = 1660(30), b_4^0 = -47(3)$		EPR	86Mal
1.993	$b_2^0 = 1650,  b_4^0  = 168, b_4^3 = 1360.8$	Nb <sup>5+</sup>	EPR	89Cho8
1.995(3)	$b_2^0 = 1815$ (3.5 K)	Li	EPR, ENDOR	92Sot
2.001(5)	$b_2^0 = 1659, b_4^0 = -900$	Li <sup>+</sup> , Nb <sup>5+</sup> , V	EPR*	93Par2
2.001(5)	$b_2^0 = 1524, b_4^0 = 0$			
2.001(5)	$b_2^0 = 1740, b_4^0 = -900$			
$g_{\parallel} = 2.019$	$b_2^0 = 1768(20), b_4^0 = -49(5)$	Li <sup>+</sup>	EPR	93Mal <sup>a)</sup>
$g_{\perp} = 1.983$	$b_4^3 = 650(50), b_4^{-3} = -380(50)$			
$g_{\parallel} = 1.984(3)$	$b_2^0 = 1640(5), b_4^0 = -54.0(6), b_4^3 = -90(12)$	Nb <sup>5+</sup>	EPR*; SPM	94Yeo1
$g_{\perp} = 1.992(3)$	$b_4^{-3} = 2022(36)$		calculation	

<sup>a)</sup> FeI centre observed in EPR spectra at 25 K after reduction of a stoichiometric LiNbO<sub>3</sub> sample grown from melts containing 6 wt% K<sub>2</sub>O.

<sup>b)</sup> rest Li<sup>+</sup>

**Table 2A-1-032.** LiNbO<sub>3</sub>:Mn<sup>2+</sup>. Spin-Hamiltonian parameters and proposed site assignment for Mn<sup>2+</sup> [94Yeo2].

$g$	FS [ $\cdot 10^{-2} \text{ m}^{-1}$ ]	Site	Method	Ref.
1.995(5)	$b_2^0 = 726(6), b_4^0 = -2(2), b_4^3 = 0$	Li <sup>+</sup>	EPR*	68Dan
$g = 1.998(2)$	$b_2^0 = 711(8), b_4^0 = -8(6)$	Nb <sup>5+</sup>	EPR	69Pet
1.998	$b_2^0 = 732, b_4^0 = -1.08,  b_4^3  = 960$		EPR	72Rex
$g_{\parallel} = 2.0002(5)$	$b_2^0 = 725, b_4^0 = -2.5(15)$	Li <sup>+</sup> or Nb <sup>5+</sup>	EPR*	72Her
1.998	$b_2^0 = 783, b_4^0 = -1.20,  b_4^3  = 1020$	Nb <sup>5+</sup>	EPR	83Mal
1.998	$b_2^0 = 735, b_4^0 = -1.14, b_4^3 = 960$	Li <sup>+</sup>	EPR*	85Mal, 89Gli
1.998(1)	$b_2^0 = 730(5), b_4^0 = -2.49$	Li <sup>+</sup>	EPR*	68Tak
2.006	$b_2^0 = 731, b_4^0 = -2.0, b_4^3 = 941$	Nb <sup>5+</sup>	EPR*, NMR	89Cho8, 91Yeo
$g_{\parallel} = 1.997(3)$	$b_2^0 = 724.5(9), b_4^0 = -0.72(1), b_4^3 = -9.4(2)$	Nb <sup>5+</sup>	EPR*; SPM	94Yeo2
$g_{\perp} = 2.009(1)$	$b_4^{-3} = 684.0(1)$		calculation	

**Table 2A-1-033.** LiNbO<sub>3</sub>. Phonon frequencies at Brillouin zone center and zone boundary [78Cho]. Frequencies are in THz.

Neutron measurements				Optical measurements [67Bar]	
$q = (0,0, 3\pi/c)$		$q = 0$		$q \cong 0$	
Frequency	Symmetry	Frequency	Symmetry	Frequency	Symmetry
4.0(8)	$\Lambda_3$	4.55(10)	$\Gamma_3$	4.50	E(T)
		7.3 <sup>a)</sup>	$\Gamma_3$	7.14	E(T)
				7.95	E(T)
		10.0(1)	$\Gamma_3$	9.63	E(T)
				10.0	E(L)
		6.70(15)	$\Gamma_2$		
5.70(15)	$(\Lambda_1+\Lambda_2)$			7.56	A <sub>1</sub> (T)
		7.85(15)	$\Gamma_1$	8.19	A <sub>1</sub> (L)
8.10(10)	$(\Lambda_1+\Lambda_2)$			8.23	A <sub>1</sub> (T)
		9.42(25)	$\Gamma_2$		
		13.65(15)	$\Gamma_2$	10.0	A <sub>1</sub> (T)
13.88(25)	$(\Lambda_1+\Lambda_2)$				
		13.90(25) <sup>b)</sup>	$\Gamma_1$	12.69	A <sub>1</sub> (L)

<sup>a)</sup> Extrapolated from about halfway between zone center and zone boundary.<sup>b)</sup> Less reliable data than others.

**Table 2A-1-034.** LiNbO<sub>3</sub> (doped). Summary of EXAFS spectra [92Zal].  $N$ : coordination number;  $R$ : neighbor distance;  $\sigma$ : Debye-Waller disorder parameter;  $\delta$ : shift from the center of the oxygen octahedron,  $\Gamma$ : constant related to the mean free path of the photoelectron.

Ion	Pair	$N$	$R$ [Å]	$\sigma^2$ [Å <sup>2</sup> ]	$\Gamma$ [Å <sup>-2</sup> ]	$\delta$ [Å]
Ni <sup>2+</sup>	Ni–O	6	2.01	0.08	1.8	0
	Ni–Nb	6	3.1	0.09	1.8	
Fe <sup>3+</sup>	Fe–O	3	2.041	0.086	1.0	–0.5
	Fe–O	3	2.298	0.105	1.0	
	Fe–Nb	4	3.199	0.06	1.0	
	Fe–Nb	3	3.398	0.049	1.0	
Ti <sup>4+</sup>	Ti–O	6	1.97	0.08	1.9	0
	Ti–Nb	7	3.18	0.06	1.9	
Hf <sup>4+</sup>	Hf–O	6	2.065	0.094	2.2	0
	Hf–Nb	1	2.57	0.089	2.2	
	Hf–Nb	6	3.30	0.085	2.2	
Ta <sup>5+</sup>	Ta–O	3	1.93	0.08	4.75	+0.25
	Ta–O	3	1.99	0.08	4.75	
	Ta–Nb	6	3.68	0.09	4.75	
Er <sup>3+</sup>	Er–O	6	2.00	0.067	2.8	0
	Er–Nb	4	3.05	0.105	2.8	
	Er–Nb	3	3.60	0.022	2.8	
Nd <sup>3+</sup>	Nd–O	6	2.03	0.077	2.0	0
	Nd–Nb	6	3.65	0.082	2.0	

**Table 2A-1-035.** LiNbO<sub>3</sub>. Diffusion coefficients of impurities [82Gon].  $D_{\parallel}$ ,  $D_{\perp}$  are the coefficients for diffusion parallel and perpendicular to the  $c$  axis, respectively.  $E$ : activation energy parallel to the  $c$ -axis.

Ion	$T$ [K]	$D_{\parallel}$ [m <sup>2</sup> s <sup>-1</sup> ]	$D_{\perp}$ [m <sup>2</sup> s <sup>-1</sup> ]	$E$ [eV]
D	873	$4.5 \cdot 10^{-12}$	$5 \cdot 10^{-12}$	1.4
O	1273	$1.0 \cdot 10^{-16}$		1.2
Li	1373	$1.5 \cdot 10^{-13}$	$4.2 \cdot 10^{-13}$	
Mg	1273		$4.5 \cdot 10^{-16}$	1.4
Ti	1273		$4.6 \cdot 10^{-17}$	2.2
Ti, V, Ni	1233	$3 \dots 23 \cdot 10^{-17}$	$1.4 \cdot 10^{-17}$	

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