## No. 1A-5 $KTaO_3$, Potassium tantalate

($M$ = 268.04)

1a Ferroelectric activity was reported by Matthias in 1949 [a]), but Wemple has proved that the ferroelectric transition does not occur in pure crystal at least above 1.6 K [b]). It is known that the ferroelectric-like activity is induced by uniaxial stress or very low level doping of impurities on either K or Ta site. [a]) 49Mat1, 49Mat2 [b]) 64Wem, 65Wem

See 92Gli

b

| | |
|---|---|
| state | P |
| crystal system | cubic |
| space group | $Pm3m - O_h^1$ |

64Wem, 65Wem, 51Vou1

$T_{melt}$ = 1357(3) °C. 55Rei, 56Rei

$\rho$ = 6.97·10³ kg m⁻³. 58Rei

Transparent, colorless or pale blue (blue in oxygen-deficient crystals). 64Win

Cleavage plane: (100).

$\Theta_f$ vs. x in $K_{1-x}Li_xTaO_3$ ($x \leq 0.08$): Fig. 1A-5-001.

2a Crystal growth:

Flux method: KF, dark small crystals [a]); $K_2CO_3$, large (≈ 10 mm) transparent crystals [b]). [a]) 62Tim, 64Wem [b]) 66Uno

Czochralski-Kyropoulos method: large (≈ 10 mm) good quality crystals. 64Wem, 65Wem, 67Bon

Floating technique: planar single crystals. 66Wil

Phase diagram of $K_2CO_3 - Ta_2O_5$ system: Fig. 1A-5-002.

Hydrothermal phase diagram $K_2O - Ta_2O_5 - H_2O$ at 400 °C: see 67Mar

3a $a$ = 3.9885 Å at RT. 51Vou1

b $Z$ = 1.

Crystal structure: cubic perovskite type; see 51Vou1, 51Vou2

K at 1a position; Ta at 1b position; 3O at 3c position.

4 Temperature dependence of lattice parameter: Figs. 1A-5-003, 1A-5-004, 1A-5-005.

Linear thermal expansion coefficient below 30 K: Fig. 1A-5-006.

5a Dielectric constant at low frequencies: earlier studies showed a peak in the $\kappa$ vs. $T$ curve [a]); measurements have shown that no peak exists down to 1.6 K [b]). [a]) 50Hul [b]) 65Wem, 64Wem

Figs. 1A-5-007, 1A-5-008, 1A-5-009, 1A-5-010, 1A-5-011, 1A-5-012.

Arrhenius plot: Fig. 1A-5-013.

$\kappa$ = 243 at RT. 65Wem

$\kappa = \kappa_0 + C / (T - \Theta_p)$, $T$ > 30 K, where $\kappa_0$ = 48, $C$ = 5.7·10⁴ K, $\Theta_p$ = 4 K.

Loss tangent: $\tan\delta \approx 0.001$ at 200 kHz at RT. 64Win

Dielectric constant in MHz ... GHz range: Fig. 1A-5-14, Fig. 1A-5-15; see also 84Bel

Dielectric dispersion in Mn, Co, Ni, Fe doped $KTaO_3$: see 94Now

Dielectric loss in the far infrared frequency range: see subsubsection 9a (Fig. 1A-5-045, Fig. 1A-5-046, Fig. 1A-5-047).

| | | |
|---|---|---|
| | Effect of hydrostatic pressure on $\kappa$: Figs. 1A-5-016, 1A-5-017, 1A-5-018.<br>Effect of uniaxial stress on $\kappa$: Figs. 1A-5-019, 1A-5-020, 1A-5-021.<br>Effect of magnetic field on $\kappa$: Fig. 1A-5-022; see also | 85Law |
| b | Effect of dc bias field on $\kappa$: Figs. 1A-5-023, 1A-5-024, 1A-5-025, 1A-5-026.<br>Coefficients in free energy expansion:<br>$\xi = 9 \cdot 10^9$ $Vm^5C^{-3}$ at 4.2 K, $\xi = 4(1) \cdot 10^9$ $Vm^5C^{-3}$ at 295 K.<br>*D* vs. *E* curves show no hysteresis character down to 1.6 K.<br>*P* vs. *E*: Fig. 1A-5-027.<br>Spontaneous polarization and coercive field in $K_{0.92}Li_{0.08}TaO_3$: Fig. 1A-5-028. | 65Kah<br>65Wem |
| c | *D* vs. *E* loops on $K_{0.9}Li_{0.1}TaO_3$: see<br>Effect of uniaxial stress on *P*: see Fig. 1A-5-020. | 85Nad |
| d | Electrocaloric effect: Fig. 1A-5-029.<br>Pyroelectric properties on $K_{1-x}Li_xTaO_3$ ($0.01 < x < 0.06$): see | 83van |
| 6a | Specific heat vs. *T*: see<br>Specific heat at low temperatures: Figs. 1A-5-030, 1A-5-031, 1A-5-032.<br>Effect of intense dc bias field on $c_p$: see | 79Tsu<br>78Law |
| b | Thermal conductivity: Figs. 1A-5-033, 1A-5-034, 1A-5-035. | |
| 7b | Electrostriction constants at 4.2 K:<br>$Q_{11} = 8.7(6) \cdot 10^{-2}$ $m^4C^{-2}$, $Q_{12} = -2.3(2) \cdot 10^{-2}$ $m^4C^{-2}$, $Q_{44} = 3.0(3) \cdot 10^{-2}$ $m^4C^{-2}$,<br>which were determined from the analysis of stress dependence of $\kappa$ in the P phase. | 75Uwe,<br>77Hoc |
| 8a | Elastic properties: Fig. 1A-5-036, Fig. 1A-5-037.<br>Elastic properties on Li, Nb doped $KTaO_3$: see | 83van |
| 9a | Refractive index in visible region: Fig. 1A-5-038.<br>Refractive index vs. *T*: Fig. 1A-5-039.<br>Birefringence vs. *T* on Li doped sample under several intense dc electric fields.<br>See also | 95Ban<br>81Cou,<br>81Cor |
| | Reflection spectra in the intrinsic absorption region (3.5 eV…35 eV): see<br>Reflectivity in far infrared region and dispersion: Fig. 1A-5-040, Fig. 1A-5-041.<br>Infrared spectra due to hydroxyl ions ($OH^-$, $OD^-$, $OT^-$). | 84Mam<br>80Eng,<br>88Hou,<br>90Jov,<br>93Jan |
| | Light irradiation effects on the transmission spectra in the visible range: Fig. 1A-5-042, Fig. 1A-5-043. | |
| | Reflectivity data were used to obtain transverse optical modes of the lattice vibration by means of Kramers-Kronig relation (cf. Table 1A-5-001).<br>Temperature dependence of the low transverse optical modes t1, t2, t3: Table 1A-5-001; Fig. 1A-5-044. | 63Mil,<br>67Per |
| | The square of the frequency $\nu_{t1}$ for the "ferroelectric mode" is approximately linear to *T*: $\nu_{t1}^2 \propto (T - \Theta_p)$. (Additional data are given on the ferroelectric soft mode, see subsubsection 14b.) | 67Per,<br>67Fle |
| | Effect of lattice vibration on the fluorescent spectrum of $Eu^{3+}$ in $KTaO_3$: see<br>Dielectric constant in the far infrared region: Figs. 1A-5-045, 1A-5-046, 1A-5-047.<br>Absorption coefficient $\alpha$ depends on the degree of oxygen reduction in $KTaO_3$.<br>Absorption coefficient near the interband absorption edge (about 3.6 eV) for insulating and semiconducting $KTaO_3$: Fig. 1A-5-048.<br>Absorption vs. wavelength of light: Fig. 1A-5-049, Fig. 1A-5-050. | 65Sch<br>65Wem |

| | | |
|---|---|---|
| | Absorption vs. carrier concentration in semiconducting $KTaO_3$: Fig. 1A-5-051.<br>Optical absorption in impurity doped single crystal: for impurities Fe, Mn, Co and Cr, see | 64Wem |
| b | Quadratic electrooptic constants (632.8 nm, 2...77 K):<br>$M_{11} - M_{12} = 0.16(1)\ m^4C^{-2}$; $M_{44} = 0.12(1)\ m^4C^{-2}$.<br>$M_{11} \approx 0.25\ m^4C^{-2}$ for $h\nu = 4$ eV at RT. | 64Geu, 63Geu 67Fro |
| | Electroreflectance and electroabsorption were studied using semiconducting $KTaO_3$.<br>Effect of interface dc field on the reflectance of the (100) surface: Fig. 1A-5-052.<br>Electroreflectance spectra of (100) and (111) surfaces: Fig. 1A-5-053, Fig. 1A-5-054.<br>Effect of polarization of light on the electroreflectance: Fig. 1A-5-055.<br>Electroreflectance as a function of the surface polarization: Fig. 1A-5-056.<br>Electroreflectance singularities and the corresponding energies: Table 1A-5-002.<br>Electroabsorption near the absorption edge: Fig. 1A-5-057.<br>Fundamental absorption edge (≈ 3.6 eV) shifts to higher energies with dc bias: Fig. 1A-5-058. | 67Fro |
| c | SHG efficiency vs. $T$ on Li doped $KTaO_3$: see | 84Gra, 95Ban |
| | Two photon absorption spectra in the edge absorption region (3.9 eV…4.4 eV): Fig. 1A-5-059. | |
| d | Faraday rotation near the band edge: Fig. 1A-5-060; see also | 67Bae, 66Bae |
| e | Nonlinear optical properties: Fig. 1A-5-061, Fig. 1A-5-062. | |
| 10a | Raman scattering: Figs. 1A-5-063, 1A-5-064, 1A-5-065, 1A-5-066. | |
| | Raman scattering spectra of n-type $KTaO_3$ ($n = 10^{24}…10^{25}\ m^{-3}$): see | 80Uwe, 83Uwe |
| | See also | 86Uwe, 85Uwe |
| | Spin-flip Raman scattering on n-type $KTaO_3$ in magnetic fields: see | 84Dou |
| | Raman spectra of $K_{1-x}Li_xTaO_3$ ($0.002 < x < 0.054$): see | 81Pra1, 96Cal |
| | Raman spectra of $KTa_{1-x}Nb_xO_3$: Fig. 1A-5-067.<br>Hyper Raman scattering: Figs. 1A-5-068, 1A-5-069, 1A-5-070, 1A-5-071; Table 1A-5-003; see also | 84Vog |
| b | Central peak: Fig. 1A-5-072. | |
| 11 | Resistivity of insulating single crystal: $\rho > 10^8\ \Omega m$ at RT.<br>Resistivity of oxygen-deficient single crystal as a function of temperature: Fig. 1A-5-073.<br>Electrical conductivity vs. oxygen partial pressure: Fig. 1A-5-074.<br>Electrical conductivity vs. hydrostatic pressure: Fig. 1A-5-075. | 65Wem |
| | Electrical conductivity vs. $T$ on Nb doped samples: see | 83Tan |
| | Protonic conduction in Fe-doped single crystal: see | 92Sch |
| | Photoconductivity vs. $h\nu$ shows a peak at $h\nu = 3.58$ eV. | 65Wem |
| | Photoconductivity in Li doped samples: see | 94Kle |
| | Negative differential photoconductivity and photo-Hall mobility vs. $T$: see | 79Kaw |
| | Photocurrent behavior: see | 73Pet, 76Ohi |
| | Photocurrent behavior in non-doped $KTaO_3$: see | 85Sek |

Photocurrent behavior in Fe, Ni doped $KTaO_3$: see 80Aki, 82Aki, 84Yam

X-ray photoelectron spectra: Fig. 1A-5-076.

Hall mobility vs. $T$: Fig. 1A-5-077, Fig. 1A-5-078; see also 79Tsu

Hall coefficient and Hall mobility at 4.2 K and RT for several semiconducting $KTaO_3$: Table 1A-5-004.

Hall mobility vs. carrier concentration: Fig. 1A-5-079.

Scattering cross section vs. carrier concentration: see 65Wem

Ca concentration in doped $KTaO_3$ vs. net ionized donor concentration: see 66Sen

Seebeck coefficient: 77Kaw, 79Tsu

Effective mass estimated from the Seebeck coefficient: $m^* = 0.80(28)\ m_0$.

Shubnikov-de Haas effect: see 79Nic, 79Uwe

Luminescence spectra: Fig. 1A-5-080, Fig. 1A-5-081; see also 85Sek

Photoluminescence spectra and decay curves of undoped $KTaO_3$. 88Yam

Infrared fluorescence spectra of $KTaO_3$:$Cr^{3+}$: see 85Tre, 88Tre

Electronic band structure: see 76Mic, 92Neu, 96Sin

Band gap energies determined by various methods: 67Bae, 67Fro

| Method | 296 K | 77 K |
|---|---|---|
| Faraday rotation | 3.77 eV<br>3.62 eV | 3.79 eV<br>3.65 eV |
| Electroreflectance singularities | 3.57 eV<br>3.80 eV | |
| Absorption data | 3.75 eV | |
| Energy at $\alpha \approx 10^6\ m^{-1}$ | 3.79 eV | |

Cyclotron resonance of semiconducting $KTaO_3$ at 70 GHz and 1.4 K; microwave skin depth: about 30 μm. 65Sen

Electron tunneling experiments: d-band width ≈ 6.8 eV, effective mass = 0.69(1) $m_0$. 70Sro

13a NMR of $^{181}Ta$ in $KTaO_3$: spin-lattice relaxation time, $T_1 \approx 10^{-3}$ s at RT; spin-spin relaxation time, $T_2 \approx 10^{-5}$ s at RT; nuclear magnetic moment of $^{181}Ta$ ($I = 7/2$): $p_n = 2.340(1)\ \mu_n$ (uncorrected); ($p_n = 2.35(1)\ \mu_n$, after estimated corrections). 60Ben

Nuclear magnetic acoustic resonance: the absorption data are given for $\Delta m = 2$ transition of $^{181}Ta$ as a function of the angle between magnetic field and sound axis [100]; see also 67Meb, 68Gre

NMR of $^7Li$, $^{39}K$ and $^{181}Ta$ in Li doped $KTaO_3$: see 84Bor, 84van

b ESR of $Eu^{2+}$, $Gd^{3+}$ and $Ti^{3+}$ in $KTaO_3$: Table 1A-5-005; see also 66Uno

ESR of $Fe^{3+}$: 83Byk, 85Gli, 94Sal, 95Lag

See also 95Rey

ESR of cubic $Fe^{3+}$ center: $a$ vs. $T$, $a$ vs. $p$ and $a$ vs. x in $KTa_{1-x}Nb_xO_3$: Fig. 1A-5-082.

ENDOR spectra: see 87Lag

| | | |
|---|---|---|
| | ESR Stark effect for $Fe^{3+}$: $E_{bias}$ along [100] induces axial splitting term $D$ ($D = 12 \cdot 10^{-2}$ m$^{-1}$ at $E_{bias} = 1.0$ MVm$^{-1}$ at 4.2 K; $D \propto E_{bias}^2$); Fig. 1A-5-083. | 63Wem, 64Wem |
| | ESR of $Ni^{3+}$ located on $Ta^{5+}$ site (low spin state) and on $K^{1+}$ site: see | 67Han |
| | ESR of $Mn^{2+}$ in $KTaO_3$ under an electric field: see | 75Dei |
| | ESR of $Gd^{3+}$ in $KTaO_3$ under an electric field: see | 82Gei, 88Gei |
| | ESR linewidth of axial $Mn^{2+}$ center vs. $T$: see | 80Byk |
| | ESR linewidth vs. Li concentration in $KTaO_3$:Li: see | 85Vug |
| | Variation of ESR line-intensity of axial $Ni^{3+}$ center (Ta site) with time, under light illumination: Fig. 1A-5-084. | |
| | Spin Hamiltonian parameters of various impurities: Tables 1A-5-006, 1A-5-007, 1A-5-008. | |
| | See also | 95Pec |
| 14b | Phonon dispersion relation for the transverse optical branch: Fig. 1A-5-085; Table 1A-5-009. | |
| | The square of the phonon energy of the ferroelectric soft mode can be approximated by $(h\nu)^2 = 10^4 A/\kappa$, 40 K < $T$ < 295 K, where $A = 2.825$ (meV)$^2$, $\kappa(T)$ is the dielectric constant. | 67Shi |
| | Neutron inelastic scattering; dispersion curves: Figs. 1A-5-086, 1A-5-087, 1A-5-088. | |
| | Neutron inelastic scattering; scattering profile: Fig. 1A-5-089, Fig. 1A-5-090. | |
| | Neutron inelastic scattering on pure, 1% Li-doped and 5% Li-doped $KTaO_3$: Temperature dependence of zone-center and zone-boundary modes: Fig. 1A-5-091. For the ferroelectric soft mode, see also subsubsection 9a. | 96Kle |
| | X-ray diffuse scattering: see | 71Com |
| | X-ray diffuse scattering on $KTaO_3$:Li and $KTaO_3$:Nb: see | 85And |
| | Relative displacements of atoms corresponding to the lowest frequency long wavelength transverse optic phonon, see | 70Har, 89Per |
| 16 | Etchant: single crystal is slowly etched by dilute HF. | 64Wem |

**Table 1A-5-001.** $KTaO_3$. Transverse optical modes at various temperatures [67Per]. The wave number $\nu_{t1}/c$ (ferroelectric soft mode) is temperature dependent.

| $T$ | $\nu_{t1}/c$ | $\nu_{t2}/c$ | $\nu_{t3}/c$ |
|---|---|---|---|
| [K] | [$\cdot 10^2$ m$^{-1}$] | | |
| 12 | 25 | 196 | |
| 126 | 58 | 198 | 551 |
| 232 | 79 | 198 | 551 |
| 295 | 88 | 199 | 550 |
| 463 | 106 | 199 | |

**Table 1A-5-002.** $KTaO_3$ (Ca-doped). Singularities observed in electroreflectance spectra (in eV) [67Fro].

| | $E_1$ | $E_2$ | $A_1$ | $A_1'$ | $A_2$ |
|---|---|---|---|---|---|
| | [eV] | | | | |
| $KTaO_3$ (100) | 3.57 | 3.80 | 4.40 | 4.88 | 5.50 |
| $KTaO_3$ (111) | | 3.77 | 4.45 | 4.90 | 5.47 |
| $KTaO_3$ (110) | 3.55 | 3.80 | 4.47 | 4.85 | 5.50 |

**Table 1A-5-003.** $KTaO_3$. Frequency, linewidth and oscillator strength at RT (unless otherwise noted) obtained by hyper-Raman scattering (HR: [84Vog]), infrared spectrum (IR: [69Per] and [63Mil]) and electric field induced Raman spectrum (R: [68Fle]).

| Mode | Symmetry | Frequency [$cm^{-1}$] | | | Linewidth, FWHM [$cm^{-1}$] | | | Oscillator strength [contribution to $\kappa(0)$] | |
|---|---|---|---|---|---|---|---|---|---|
| | | HR | IR | R | HR | IR | R | HR | IR |
| TO1 | $F_{1u}$ | 81 | 88 | 85 | 20 | 51; 47 | 20 | 233 | 209.4; 163 |
| LO1 | | 185 | 184 | | < 6 | | | | |
| TO2 | $F_{1u}$ | 199 | 199 | 198 (10 K) | < 6 | 2.4; 11 | | 6.5 | 5.0; 7.6 |
| LO2 | $F_{2u}$ | 279 | | | | | | | |
| TO3 | $F_{2u}$(silent) | 279 | | | | | | | |
| LO3 | | 422 | 421 | | 7 | | | | |
| TO4 | $F_{1u}$ | 546 | 547 | 556 (10 K) | 15 | 24 | | 2.5 | 2.4 |
| LO4 | | 826 | 838 | | 20 | | | | |

**Table 1A-5-004.** $KTaO_3$ (reduced). Hall coefficient $R_H$ and Hall mobility $\mu_H$ at 295 K and 4.2 K for single crystals [65Wem]. Carrier concentrations $N$ are calculated from the Hall coefficient at 4.2 K using $R_H = -1/Ne$.

| Sample no. | $N_{calc}$ [$m^{-3}$] | $R_H$ [$m^3C^{-1}$] | | $\mu_H$ [$m^2V^{-1}s^{-1}$] | |
|---|---|---|---|---|---|
| | | $T$ = 295 K | $T$ = 4.2 K | $T$ = 295 K | $T$ = 4.2 K |
| *1* | $3.5\cdot10^{23}$ | $20.3\cdot10^{-6}$ | $18\ \cdot10^{-6}$ | $2.7\cdot10^{-3}$ | 2.3 |
| *2* | $6.0\cdot10^{23}$ | $12.9\cdot10^{-6}$ | $10.4\cdot10^{-6}$ | $2.9\cdot10^{-3}$ | 1.9 |
| *3* | $6.6\cdot10^{23}$ | $11.5\cdot10^{-6}$ | $9.4\cdot10^{-6}$ | $3.1\cdot10^{-3}$ | 1.9 |
| *4* | $2.4\cdot10^{24}$ | $3.0\cdot10^{-6}$ | $2.6\cdot10^{-6}$ | $3.0\cdot10^{-3}$ | 1.1 |
| *5* | $7.8\cdot10^{24}$ | $1.0\cdot10^{-6}$ | $0.80\cdot10^{-6}$ | $3.0\cdot10^{-3}$ | 0.53 |
| *6* | $1.3\cdot10^{25}$ | $0.62\cdot10^{-6}$ | $0.48\cdot10^{-6}$ | $3.1\cdot10^{-3}$ | 0.34 |

**Table 1A-5-005.** $KTaO_3$. Parameters of ESR spectrum of $Eu^{2+}$, $Gd^{3+}$ and $Ti^{3+}$ ions, doped in single crystals [66Uno, 78Gei].

| Para-magnetic center | Site | $S$ | **H** | $\nu$ [GHz] | $T$ [K] | $g$-factor | FS $b_{40}$, $b_{60}$ [$\cdot 10^{-2}$ m$^{-1}$] | HFS $I$ | HFS $A$ [$\cdot 10^{-2}$ m$^{-1}$] | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|
| $Eu^{2+}$ | $K^+$ | 7/2 | (8) | 9.1 | 77 | 1.990(2) | $b_{40}$ = (±)16(2) | 5/2 | $\lvert^{151}A\rvert$ = 36(1) | 66Uno |
| | | | | | | | $b_{60}$ = (±) 1.2(6) | 5/2 | $\lvert^{153}A\rvert$ = 16(1) | |
| $Gd^{3+}$ | | 7/2 | | | 4.2 | 1.990(2) | $b_{40}$ = –8.14(27) | | | |
| | | | | | | | $b_{60}$ = +0.47(30) | | | |
| | | | | | 77 | 1.990(2) | $b_{40}$ = –7.0(3) | | | |
| | | | | | | | $b_{60}$ = +0.5(5) | | | |
| $Ti^{3+}$ | $Ta^{5+}$ | 1/2 | | | 77 | 1.997(3) | | 5/2 | $\lvert^{47}A\rvert$ = 10.8(3) | 78Gei |
| | | | | | | 1.904(3) | | 7/2 | $\lvert^{49}A\rvert$ = 11.4(3) | |

**Table 1A-5-006.** $KNbO_3$. Spin Hamiltonian parameters for $Cu^{2+}$ at 77 K [85Byk].

| | $g_{\parallel}$ | $g_{\perp}$ | $A_{\parallel}$ [$m^{-1}$] | $A_{\perp}$ [$m^{-1}$] |
|---|---|---|---|---|
| Spectrum I | 2.238(1) | 2.045(1) | $172(1)\cdot10^{-2}$ | $30(5)\cdot10^{-2}$ |
| Spectrum II | 2.194(1) | 2.045(2) | $193(1)\cdot10^{-2}$ | $\lesssim 30\cdot10^{-2}$ |

*Note*: The intensities of the lines in the spectrum II are approximately 3 times less than the intensities of the lines in the spectrum I.

**Table 1A-5-007.** $KTaO_3$. Spin Hamiltonian parameters for various impurity centers [84Abr].

| Ion | $g_{\parallel}$ | $g_{\perp}$ | FS [$\cdot 10^{-2}$ m$^{-1}$] | HFS [$\cdot 10^{-2}$ m$^{-1}$] | $T$ [K] |
|---|---|---|---|---|---|
| $Yb^{3+}$ | 4.775(2) | 2.430(1) | | $^{171}A(1/2) = 1252.2(3)$, $^{171}A(1/2) = 624.8(3)$ | 4.2 |
| | | | | $^{173}A(5/2) = 345.2(3)$, $^{173}A(5/2) = 172.7(2)$ | 4.2 |
| $U^{5+}$ | $g_{iso} = 0.616(2)$ | | | | 77 |
| $Cu^{2+}$ | 2.228(2) | 2.056(5) | | $^{65}A(3/2) = 173(2)$, $^{65}A(3/2) = 45(3)$ | 77 |
| $Co^{2+}$ | 2.067(1) | 4.958(2) | | $^{59}A(7/2) = 58.2(2)$, $^{59}A(7/2) = 73.7(3)$ | 4.2 |
| $Mn^{2+}$ | 1.9978(5) | 2.0004(5) | $b_{20} = +1480(1)$<br>$b_{40} = -1.2(4)$<br>$b_{44} = +2(2)$ | $^{55}A(5/2) = 85.9(4)$, $^{55}A(5/2) = 82.7(4)$ | 77 |
| $Ni^{3+}$ I | 2.219(1) | 4.430(2) | | | 77 |
| $Ni^{3+}$ II | 2.236(2) | 2.116(2) | | | 77 |
| $Fe^{3+}$ | 1.997(1) | 6.007(6) | | | 77 |
| $Fe^{3+}$ or $Ni^{3+}$ III | 1.968(2) | 4.337(2) | | | 77 |

**Table 1A-5-008.** $KTaO_3$, $K_{1-x}Li_xTaO_3$. Spin Hamiltonian parameters for various impurity centers [95Lag, 92Gli, 67Han]. $Fe^{3+}_{ax}(K)$: $Fe^{3+}$axial symmetry centers substituted for $K^+$, $Fe^{+}_{ax}(K)$: $Fe^+$ axial symmetry centers substituted for $K^+$, $Gd^{3+}_{c}$ : $Gd^{3+}$ cubic symmetry centers for $K^+$, $Fe^{3+}_{c}(K)$ : $Fe^{3+}$cubic symmetry centers for $K^+$, $Ni^{3+}_{c}(Ta)$ : $Ni^{3+}$ cubic symmetry centers for $Ta^{5+}$.

| Paramagnetic center | $T$ [K] | $g$-factor | FS [$\cdot 10^{-4}$ cm$^{-1}$] |
|---|---|---|---|
| **$KTaO_3$** | | | |
| $Fe^{3+}_{ax}(K)$ | 5 | $g_{\parallel} = 1.997(2)$ | |
| | | $g_{\perp} = 6.005(2)$ | |
| $Fe^{+}_{ax}(K)$ | 5 | $g_{\parallel} = 2.00(2)$ | |
| | | $g_{\perp} = 4.33(1)$ | |
| $Gd^{3+}_{c}$ (K) | 5 | 1.990(1) | $b_4 = -7.25(2)$ |
| | | | $b_6 = 0.46(2)$ |
| **$K_{1-x}Li_xTaO_3$** | | | |
| $Fe^{3+}_{ax}(K)$ | 5 | $g_{\parallel} = 1.997(2)$ | |
| | | $g_{\perp} = 6.005(2)$ | |
| $Fe^{3+}_{c}(K)$ | 5 | 1.990(2) | $b_4 = 19(1)$ |
| $Ni^{3+}_{c}(Ta)$ | 5 | 4.28(1) | |

**Table 1A-5-009.** $KTaO_3$. Phonon frequency of the soft ferroelectric mode (transverse optical mode) at various temperatures [67Shi]. The wave vector $q$ at the zone boundary is 0.788 $Å^{-1}$ (= $\pi/a$).
See Fig. 1A-5-087.

| $T$ | Phonon frequency [$\cdot 10^{12}$ Hz] | | |
|---|---|---|---|
| [K] | $q$ = 0 $Å^{-1}$ | $q$ = 0.1 $Å^{-1}$ | $q$ = 0.2 $Å^{-1}$ |
| 295 | 2.6 | 2.8 | 3.3 |
| 230 | 2.3 | | |
| 170 | 2.1 | 2.4 | 3.0 |
| 120 | 1.8 | | |
| 77 | 1.4 | 1.8 | 2.6 |
| 40 | 1.0 | 1.5 | |
| 28 | 0.9 | 1.4 | 2.5 |
| 15 | 0.8 | 1.3 | |
| 10 | 0.8 | 1.3 | |
| 4 | 0.8 | 1.3 | 2.4 |

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