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THE MOLECULAR-BEAM ELECTRIC-RESONANCE SPECTRA OF LiF, LiCl, AND KCl*

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ABSTRACT

The molecular-beam electric-resonance method has been used to observe the radio-frequency spectra of ${}^6\text{Li}^{19}\text{F}$, ${}^7\text{Li}^{19}\text{F}$, ${}^6\text{Li}^{35}\text{Cl}$, ${}^6\text{Li}^{37}\text{Cl}$, ${}^{39,35}\text{K}^{35}\text{Cl}$, and ${}^{39,37}\text{K}^{37}\text{Cl}$ in low vibrational and rotational states. Microwave $J = 1 \rightarrow 0$ transitions have also been observed for ${}^6\text{Li}^{35}\text{Cl}$ and ${}^6\text{Li}^{37}\text{Cl}$. Analysis of the spectra has given dipole moments and other molecular constants of these molecules.

I. INTRODUCTION

Previous reports from this laboratory have described the radio-frequency and microwave spectra of LiBr, ${}^1\text{LiI}$,² and NaF,³ by the molecular-beam electric-resonance method. The spectrometer used in these experiments has demonstrated high-resolution, even at strong Stark fields, and this has made possible an accurate determination of electric dipole moments, as well as rotational and nuclear hyperfine interaction constants.

The present work is a continuation of the high-resolution molecular-beam electric-resonance studies of the alkali halides. Radio-frequency Stark spectra produced by transitions of the type $(J, m_J \pm 1) \rightarrow (J, m_J)$ have been observed for the low vibrational and rotational states of ${}^6\text{Li}{}^{19}\text{F}$, ${}^7\text{Li}{}^{19}\text{F}$, ${}^6\text{Li}{}^{35}\text{Cl}$, ${}^6\text{Li}{}^{37}\text{Cl}$, ${}^{39}\text{K}{}^{35}\text{Cl}$, and ${}^{39}\text{K}{}^{37}\text{Cl}$. Microwave $J = 1 \rightarrow 0$ transitions have also been observed for ${}^6\text{Li}{}^{35}\text{Cl}$ and ${}^6\text{Li}{}^{37}\text{Cl}$.

II. EXPERIMENTAL TECHNIQUES

The electric-resonance spectrometer has been discussed in detail elsewhere^{1,4} and only a brief description will be given here. The apparatus consists of a four-chamber high-vacuum system with two 30-cm dipole inhomogeneous electric deflecting fields and a 25 cm homogeneous electric Stark-field region. The source oven is a 20% iridium-80% platinum tube with a source slit 6 mm high by 0.13 mm wide. Detection is by surface ionization on a tungsten ribbon with the positive

ions being accelerated out of the main chamber, through a mass-analyzing magnet, and into a 14-stage electron multiplier.

The Stark field is produced by parallel electrodes which were made by evaporating an aluminum film on glass optical flats. The field is parallel to $1/8 \lambda$ of helium light for a 1-cm gap or approximately 1 part in 10^5 along the 25-cm transition region. An improved voltage and field-monitoring system⁵ was used for the ${}^6\text{Li}{}^{19}\text{F}$ spectra. This reduced the electric field uncertainty to 2 parts in 10^5 with a reproducibility of the field an order of magnitude better. Since magnetic effects could be expected to produce noticeable perturbations, care was taken to reduce all components of the earth's magnetic field and fringe magnetic fields to less than 50 mG along the transition region.

The radio-frequency experiments reported here are of the "flop-in" type and require that molecules undergo a transition in order to reach the detector. Radio-frequency is applied across one of the Stark-field electrodes to induce transitions which are then observed as increases of the beam signal at the detector. The $J = 1 \rightarrow 0$ microwave transitions are observed by setting the Stark field and radio-frequency to give a maximum $(1, \pm 1) \rightarrow (1, 0)$ "flop-in" signal. Microwave frequency introduced via a horn with the microwave electric field parallel to the Stark field is then swept and a transition is observed as a decrease in the signal due to depletion of the $(1, 0)$ state because of transitions of the type $(1, 0) \rightarrow (0, 0)$.

III. THEORY

The Hamiltonian for analyzing the electric-resonance spectrum of a polar diatomic molecule in a $^1\Sigma$ electronic ground state is^{6,7}:

$$\begin{aligned}
 \mathcal{H} = & B\underline{J}^2 - \underline{\mu} \cdot \underline{E} - eq_1q_1 \frac{[3(\underline{I}_1 \cdot \underline{J})^2 + \frac{3}{2}(\underline{I}_1 \cdot \underline{J}) - (\underline{I}_1^2 \underline{J}^2)]}{2I_1(2I_1-1)(2J-1)(2J+3)} \\
 & - eq_2q_2 \frac{[3(\underline{I}_2 \cdot \underline{J})^2 + \frac{3}{2}(\underline{I}_2 \cdot \underline{J}) - (\underline{I}_2^2 \underline{J}^2)]}{2I_2(2I_2-1)(2J-1)(2J+3)} + c_1(\underline{I}_1 \cdot \underline{J}) + c_2(\underline{I}_2 \cdot \underline{J}) \\
 & + c_3 \frac{[3(\underline{I}_1 \cdot \underline{J})(\underline{I}_2 \cdot \underline{J}) + 3(\underline{I}_2 \cdot \underline{J})(\underline{I}_1 \cdot \underline{J}) - 2(\underline{I}_1 \cdot \underline{I}_2)J(J+1)]}{(2J-1)(2J+3)} + c_4(\underline{I}_1 \cdot \underline{I}_2)
 \end{aligned}$$

The first term in the above expression represents the rotation of the molecule, where B is the molecular rotational constant and \underline{J} is the rotational angular-momentum operator. The second term gives the interaction of the permanent electric dipole moment, $\underline{\mu}$, with the applied external field, \underline{E} . The third and fourth terms represent the interaction of the nuclear electric quadrupole moments (Q_1 and Q_2) with the electric field gradients at the nuclei (q_1 and q_2), where e is the electronic charge, I_1 and I_2 are the nuclear spins, and eq_1Q_1 and eq_2Q_2 are the quadrupole coupling constants. The fifth and sixth terms represent the magnetic coupling of the nuclear spins with the molecular angular momentum, where c_1 and c_2 are the spin-rotation interaction constants. The seventh and eighth terms represent the tensor and scalar spin-spin interactions, respectively. The tensor spin-spin interaction constant, c_3 , is defined as $c_3(\text{dir}) + c_3(\text{ind})$.

The direct spin-spin interaction constant, $c_3(\text{dir})$, arises from the usual magnetic dipole-dipole interaction between the two nuclei, and equals $g_1 g_2 \mu_N^2 \langle 1/r^3 \rangle$, where g_1 and g_2 are the nuclear g factors for the two nuclei, r is the internuclear distance, and μ_N is one nuclear magneton. The $\langle 1/r^3 \rangle$ calculation is made including the correction for the molecular vibrational effects as discussed by Ramsey.⁸ The indirect spin-spin interaction constant, $c_3(\text{ind})$, arises from the tensor component of an electron-coupled nuclear spin-spin interaction. The scalar spin-spin interaction constant, c_4 , arises solely from the scalar component of an electron-coupled nuclear spin-spin interaction.⁹

A computer program¹⁰ calculates the matrix elements of \mathcal{H} in a $(J, I_1, I_2, m_J, m_{I_1}, m_{I_2})$ representation, where m_J , m_{I_1} , and m_{I_2} are the projections of J, I_1 , and I_2 , respectively, on the direction of the field E . The program computes the energy eigenvalues by diagonalizing this matrix and then calculates the spectral line positions and intensities corresponding to the given set of input parameters according to the selection rules $\Delta m_F = 0, \pm 1, \pm 2, \dots$ where m_F is the projection of the total angular momentum on the field direction. Since m_F is a good quantum number at all field values, the matrix is diagonal in m_F . The line intensities are calculated from the matrix elements of the dipole-moment operator using the computed wave functions. The unknown parameters are varied to obtain the best fit to the observed spectra.

IV. RESULTS AND DISCUSSION

A. The Radio-Frequency Spectra of ${}^6\text{Li}^{19}\text{F}$ and ${}^7\text{Li}^{19}\text{F}$

The radio-frequency Stark spectra of ${}^6\text{Li}^{19}\text{F}$ and ${}^7\text{Li}^{19}\text{F}$ were first observed by Trischka et al.,^{11,12,13} and more recently by Gold,¹⁴ and Wharton et al.^{15,16} In the present work the resolution of the spectra is improved and a more accurate and complete set of the molecular constants of LiF can be reported.

Radio-frequency transitions of the type $(J=1, m_J = \pm 1) \rightarrow (J=1, m_J = 0)$ were observed for both ${}^6\text{Li}^{19}\text{F}$ and ${}^7\text{Li}^{19}\text{F}$. For ${}^7\text{Li}^{19}\text{F}$ $(J=2, m_J = \pm 2) \rightarrow (J=2, m_J = \pm 1)$ transitions were also observed. These transitions were observed in the low vibrational states of LiF at several Stark-field voltages.

The observed full width at half maximum (FWHM) for lines in the $J = 1$ rotational state of ${}^6\text{Li}^{19}\text{F}$ was 3.5 kHz when approximately 1200 V was applied to both state selecting A and B deflecting fields. The FWHM decreased to 2.2 kHz when the deflecting-field voltages were lowered to 600 V. Typical spectra illustrating this effect are shown in Figs. 1 and 2. The effect is attributed to velocity selection by the deflecting fields, collimator, and stop system. With low voltages applied to the A and B fields, only those molecules which spend a longer time in the A and B field regions are deflected sufficiently to pass by the beam-stop and reach the detector. Thus the low deflecting-field spectra utilize molecules from the low velocity portion of the effusion spectrum. These molecules spend more time in the Stark-field transition region and consequently give a small natural line width. The increased resolution is obtained only with a resultant loss in intensity and optimum spectra are obtained at some compromise

between intensity and line width. A typical spectrum of the type used in the ${}^6\text{Li}^{19}\text{F}$ calculations is shown in Fig. 1.

In analyzing the ${}^6\text{Li}^{19}\text{F}$ spectra, the unresolved multiplets were fitted to calculated composite line positions. These composite line positions were obtained by graphically adding component lines that had the experimental singlet line shape and calculated relative intensities. The validity of this technique was shown to be quite good by applying it to the unresolved multiplets of the ${}^7\text{Li}^{19}\text{F}$ spectra after obtaining a best fit using only the singlets.

The dipole moments were calculated from data taken at 800 V/cm for both isotopes and also at 1500 V/cm in the case of ${}^6\text{Li}^{19}\text{F}$. This latter experiment at 1500 V/cm utilized an improved voltage-measuring system and was used as a check against the earlier dipole-moment determinations. There is excellent agreement between both sets, however, only the more accurate 1500 V/cm values are given here. The dipole moments for both isotopic species of LiF have been fitted to an expression of the form:

$$\mu_v = \mu_e + \mu_I(v + 1/2) + \mu_{II}(v + 1/2)^2, \quad ,$$

where v is the vibrational quantum number.

The dipole moments and quadratic expression coefficients are given in Table I. The results give experimental verification for the expected variation of dipole moment with change in reduced mass due to isotopic substitution. The equilibrium dipole moments, μ_e , are the same, within the experimental error, for ${}^6\text{Li}^{19}\text{F}$ and

${}^7\text{Li}{}^{19}\text{F}$. The coefficients μ_{I} and μ_{II} follow the isotopic dependence as predicted by theory¹⁷ being proportional to

$$\frac{B_e}{\omega_e} \quad \text{and} \quad \left(\frac{B_e}{\omega_e}\right)^2 \quad \text{respectively.}$$

The hyperfine interaction constants of LiF are summarized in Table II. In the case of ${}^7\text{Li}{}^{19}\text{F}$, where both $J=1$ and 2 spectra were observed and fitted independently, the reported constants are a least squares average of the $J=1$ and 2 values.

The ${}^7\text{Li}{}^{19}\text{F}$ quadrupole-coupling constants were fitted to an expression linear in the vibrational quantum number. The ratio of the equilibrium quadrupole coupling constants,

$$\left[(\text{eqQ})_e\right]_{6\text{Li}} / \left[(\text{eqQ})_e\right]_{7\text{Li}} = 0.0205 \pm 0.002 \quad ,$$

is in good agreement with other reported ratios of the nuclear quadrupole moments of ${}^6\text{Li}$ to ${}^7\text{Li}$.^{16,18,19}

The spin-rotation interaction constant can be expressed as proportional to an electronic factor times $\mu_N g_n B$,²⁰ where μ_N is one nuclear magneton, g_n is the nuclear g factor and B is the rotational constant. The ratios of the lithium and fluorine spin-rotation constants for the two molecules agree with the expected isotopic variations of g_n and B . Within experimental error the fluorine spin-rotation constants, C_F , are proportional to B in the first three

vibrational states, and consequently, in contrast to Kastner et al.¹³ we find no evidence for any large change in the electronic factor.

Best fits to the observed spectra of ${}^7\text{Li}^{19}\text{F}$ were obtained by setting c_4 equal to zero and c_3 equal to the calculated $c_3(\text{dir})$. The fits obtained for the $J = 1$ spectra and especially those obtained for the $J = 2$ spectra of ${}^7\text{Li}^{19}\text{F}$ indicate that there is no experimental justification for the inclusion of c_4 in these calculations or for assigning any value other than $c_3(\text{dir})$ to c_3 . In this respect the present results differ from those of Wharton et al.,¹⁶ who give a value of 210 ± 40 cps for c_4 of Li^7F in the $V=0$ state. In all ${}^6\text{Li}^{19}\text{F}$ calculations $c_3(\text{dir})$ was used for c_3 , and c_4 is assumed equal to zero.

B. The Radio-Frequency and Microwave Spectra of ${}^6\text{Li}^{35}\text{Cl}$ and ${}^6\text{Li}^{37}\text{Cl}$.

Previous work on LiCl includes the radio-frequency studies of ${}^6\text{Li}^{35}\text{Cl}$ as reported by Marple and Trischka,²¹ and the microwave studies of ${}^7\text{Li}^{35}\text{Cl}$ and ${}^7\text{Li}^{37}\text{Cl}$ as reported by Lide, Cahill, and Gold.²² Klemperer, et al.,²³ have reported the results of an infrared analysis of ${}^7\text{LiCl}$.

In the present work the radio-frequency and microwave spectra of ${}^6\text{Li}^{35}\text{Cl}$ and ${}^6\text{Li}^{37}\text{Cl}$ have been observed. This study was concerned with radio-frequency transitions of the type $(J=1, m_J = \pm 1) \rightarrow (J=1, m_J = 0)$, and $J = 1 \rightarrow 0$ microwave transitions.

Values were obtained for the electric dipole moment, the chlorine quadrupole-interaction constants, and the chlorine spin-rotation interaction constant

in the first three vibrational states of ${}^6\text{Li}^{35}\text{Cl}$ and ${}^6\text{Li}^{37}\text{Cl}$. Observation of rotational transitions in the $v=0, 1,$ and 2 vibrational states of ${}^6\text{Li}^{35}\text{Cl}$ and the $v=0$ vibrational state of ${}^6\text{Li}^{37}\text{Cl}$, in conjunction with the ω_e and $\omega_e X_e$ values reported by Klemperer et al.,²³ allowed a determination of the Dunham coefficients Y_{01} , Y_{11} , and Y_{21} .²⁴

The nuclear quadrupole and spin-rotation interactions of the chlorine nucleus alone were found to be adequate for the interpretation of the radio-frequency observations. Our present signal-to-noise ratios and line widths of 4.5 kHz prevented the resolution of splittings and small line shifts which are expected to arise from the much smaller hyperfine interactions of the ${}^6\text{Li}$ nucleus. The ${}^6\text{Li}$ quadrupole-interaction constant, calculated from the $Q_6\text{Li}/Q_7\text{Li}$ ratio of LiF and the value of $(eqQ)_{7\text{Li}}$ given by Gold,¹⁴ is 5.13 kHz. This interaction is expected to cause splittings of the order of 2 kHz in each of the observed 6 major lines. The ${}^6\text{Li}$ spin-rotation interaction is expected to cause even smaller effects which are also unresolved. The calculated value of the magnetic dipole-dipole interaction constant is approximately 42 Hz for ${}^6\text{Li}^{35}\text{Cl}$. Initial calculations indicated that the effect of this term is negligible and it has not been used in subsequent calculations.

The FWHM of the radio-frequency lines was approximately 4.5 kHz and the signal-to-noise ratio was approximately 20 to 1 for the $v=0$ vibrational state of ${}^6\text{Li}^{35}\text{Cl}$. The $J = 1 \rightarrow 0$ microwave transitions were observed as a decrease (~50%) in the "flop-in" Stark signal, and the microwave line widths were approximately 70 kHz at transition frequencies near 48 GHz.

The dipole moments were fitted to the quadratic expression for the variation of the dipole moment with vibrational state. The dipole moments and derived

expressions are given in Table III and are compared with the previous values as calculated from the μ^2_A values reported by Marple and Trischka.²¹ The present dipole moments are significantly higher. They are expected to be accurate to ± 1 part in 10^4 and the reproducibility is an order of magnitude better. Previous determinations of the dipole moments of NaF,³ and LiF from this laboratory are in good agreement with those of other investigators.^{15,25} The ratios of the coefficients μ_I and μ_{II} for the two isotopic species of LiCl are in agreement with the expected isotopic dependence.

Table IV lists the values of $(eqQ)_{Cl}$ and c_{Cl} for ${}^6\text{LiCl}$ in the $V=0, 1,$ and 2 vibrational states and also the quadratic expression coefficients of $(eqQ)_{Cl}$. These values are in agreement with those of Marple and Trischka²¹ within the combined experimental errors.

$$[(eqQ)_e]_{35Cl} / [(eqQ)_e]_{37Cl} = 1.2679 \pm 0.0056$$

This ratio is in agreement with the more precise nuclear moment-ratio determinations by Wang, et al.²⁶

The observed microwave-transition frequencies were corrected to zero-field frequencies in the absence of all hyperfine interactions by using the molecular constants obtained from analysis of the radio-frequency Stark spectra. Centrifugal distortion constants for a given vibrational state, D_v , were calculated from the results of Klemperer, et al.²³ The Dunham coefficients, Y_{01} , Y_{11} , and Y_{21} , were determined by fitting the zero-field microwave frequencies to the expression:

$$\nu_0 = 2Y_{01} + 2Y_{11}(v + 1/2) + 2Y_{21}(v + 1/2)^2 - 4D_v$$

Table V lists values of B_e , Y_{01} , Y_{11} , Y_{21} , and B_v for ${}^6\text{Li}^{35}\text{Cl}$ and ${}^6\text{Li}^{37}\text{Cl}$. Spectroscopic constants for ${}^7\text{LiCl}$ were calculated from the present ${}^6\text{LiCl}$ results and are compared with the results of Lide, Cahill, and Gold²² in Table VI. The agreement is excellent.

C. The Radio-Frequency Spectra of ${}^{39}\text{K}^{35}\text{Cl}$ and ${}^{39}\text{K}^{37}\text{Cl}$

The electric resonance microwave spectra of KCl were observed previously by Lee, et al.,²⁷ and values were reported for the rotational constants, quadrupole-coupling constants, and dipole moments. The dipole moments were determined from weak field spectra and exhibited an anomalously large variation with vibrational state. The present work was therefore undertaken to observe strong field spectra where a more accurate determination of the dipole moment could be made.

Because of the rather small rotational constant of KCl, the $J = 1$ rotational state molecules can not be sufficiently deflected with the present experimental design. However, higher J states can be studied and the observed radio-frequency spectra were produced by transitions of the type $(2, \pm 1) \rightarrow (2, 0)$ in the low vibrational states.

A typical KCl resonance in the $v = 0$ vibrational state had a FWHM of 20 kHz and a signal-to-noise ratio of only 2 to 1. Better statistics for the observed spectra were obtained by computer addition of several runs with a resultant increase in the S/N ratio. This technique made possible the analysis of $v = 2$ spectra, not observable with a single spectral run.

The six major observed resonances of the $J = 2$ spectrum were due to the potassium quadrupole splitting of the Stark transition. There was no resolvable structure in the lines and therefore additional hyperfine interaction constants could not be determined; however, upper limits on these constants could be set by considering the line widths.

Table VII summarizes the present dipole-moment determinations and gives comparisons with those of Lee et al.²⁷ There are large differences between the two sets. The present results do not exhibit the previously observed anomalous variation of dipole moment with vibrational state.

The observed potassium quadrupole-coupling constants were in good agreement with the more accurate values reported by Lee, et al.²⁷

An upper limit of 300 kHz could be placed on the absolute value of the chlorine quadrupole coupling constant for all three vibrational states. Also an upper limit of 2 kHz could be placed on both spin-rotation interaction constants, c_K and c_{Cl} .

Table I. Dipole moments and dipole-moment functions for LiF.^a All values are given in Debyes.

	Dipole Moments	
	⁶ Li ¹⁹ F ^b	⁷ Li ¹⁹ F
μ_0	6.32736(20)	6.3248(10)
μ_1	6.41472(20)	6.4072(10)
μ_2	6.50317(20)	6.4905(10)
	Dipole Moment Functions	
	$\mu_v = \mu_e + \mu_I(v+1/2) + \mu_{II}(v+1/2)^2$	
μ_e	6.28409(25)	6.2839(12)
μ_I	0.08627(5)	0.08153(30)
μ_{II}	0.00054(2)	0.00044(12)

^aThe accuracy of the dipole moments is limited by the uncertainty in the absolute value of the electric Stark field; however, the precision of the results is at least an order of magnitude better and allows smaller errors to be reported for the coefficients in the dipole-moment expressions.

^bCalculations were made with the field in absolute units, assuming that one NBS legal volt equals 1.000011 absolute volts.

Table II. Hyperfine interaction constants for LiF. All values are given in kHz.

Vibrational state	eqQ_{Li}	c_{Li}	c_F	c_3	c_4
			${}^6_{Li}{}^{19}_F$		
$v = 0$	8.5(8)	0.71(8)	36.8(4)	4.307(8)	0.00(15)
$v = 1$	8.6(1.2)	0.71(12)	36.1(5)	4.244(12)	0.00(20)
$v = 2$	7.1(2.0)	0.73(20)	35.7(7)	4.140(20)	0.00(40)
			${}^7_{Li}{}^{19}_F$		
$v = 0$	415.6(4)	1.87(3)	32.68(16)	11.382(20)	0.00(8)
$v = 1$	406.1(6)	1.84(4)	32.20(22)	11.173(30)	0.00(11)
$v = 2$	396.5(8)	1.79(4)	31.84(24)	10.964(30)	0.00(14)

$(eqQ)_v = (eqQ)_e + (eqQ)_I(v+1/2)^2$
 $(eqQ)_e = 420.3(8)$
 $(eqQ)_I = -9.4(1.2)$

Table III. Dipole moments and dipole-moment functions for ${}^6\text{LiCl}$. All values are given in Debyes.

	Dipole Moments	
	Present results ^a	Previous results ^b
	${}^6\text{Li}{}^{35}\text{Cl}$	
μ_0	7.1289(10)	7.1195(22)
μ_1	7.2168(10)	7.2069(22)
μ_2	7.3059(10)	7.2964(22)
	${}^6\text{Li}{}^{37}\text{Cl}$	
μ_0	7.1287(10)	7.1192(22)
μ_1	7.2163(10)	7.2071(22)
μ_2	7.3052(10)	7.2972(22)
	Dipole Moment Functions	
	$\mu_v = \mu_e + \mu_I(v+1/2) + \mu_{II}(v+1/2)^2$	
	Present results ^a	
	${}^6\text{Li}{}^{35}\text{Cl}$	
μ_e	7.0853(13)	
μ_I	0.0868(4)	
μ_{II}	0.00056(14)	
	${}^6\text{Li}{}^{37}\text{Cl}$	
μ_e	7.0853(13)	
μ_I	0.0864(5)	
μ_{II}	0.00064(16)	

^aSee note a, Table I.

^bThese dipole moments were derived from the μ^2 A data given by Marple and Trischka.²¹

Table IV. Chlorine quadrupole-coupling constants, $(eqQ)_v$, and spin-rotation constants, $(C_{Cl})_v$, for ${}^6\text{LiCl}$. All values are given in kHz.

v	${}^6\text{Li}^{35}\text{Cl}$		${}^6\text{Li}^{37}\text{Cl}$	
	$(eqQ)_{Cl}$	C_{Cl}	$(eqQ)_{Cl}$	C_{Cl}
0	-3072.1(1.1)	2.34(19)	-2420.8(1.4)	1.75(23)
1	-3478.7(1.2)	2.26(20)	-2739.6(1.5)	1.82(25)
2	-3872.9(2.1)	2.26(36)	-3051.9(2.7)	1.77(45)

$$(eqQ)_v = (eqQ)_e + (eqQ)_I(v+1/2) + (eqQ)_{II}(v+1/2)^2$$

$(eqQ)_e = -2864.2(2.8)$	$(eqQ)_e = -2259.0(3.6)$
$(eqQ)_I = -419.0(3.3)$	$(eqQ)_I = -325.2(4.3)$
$(eqQ)_{II} = 6.2(2.1)$	$(eqQ)_{II} = 3.2(2.6)$

Table V. Spectroscopic constants of ${}^6\text{LiCl}$. All values are in MHz.

${}^6\text{Li}^{35}\text{Cl}$:

$$B_e = 24116.74(30)$$

$$Y_{01} = 24116.582(33)$$

$$Y_{11} (\approx \alpha_e) = -291.760(45)$$

$$Y_{21} (\approx \gamma_e) = 1.546(16)$$

$$B_0 = 23971.088(6)$$

$$B_1 = 23682.420(7)$$

$$B_2 = 23396.844(12)$$

${}^6\text{Li}^{37}\text{Cl}$:

$$B_0 = 23781.615(9)$$

Table VI. Spectroscopic constants of ${}^7\text{LiCl}$. All values are in MHz.

	lide, Cahill, and Gold ²²	Data calculated ^a from present ${}^6\text{Li}{}^{35}\text{Cl}$ results
	${}^7\text{Li}{}^{35}\text{Cl}$	
B_e		21181.27(30)
$Y_{01} (\approx B_e)$	21181.1(1)	21181.15(3)
$-Y_{11} (\approx \alpha_e)$	240.2(2)	240.15(4)
$Y_{21} (\approx \gamma_e)$	1.2(2)	1.19(1)
	${}^7\text{Li}{}^{37}\text{Cl}$	
B_e		20990.05(30)
$Y_{01} (\approx B_e)$	20989.9(1)	20989.87(3)
$-Y_{11} (\approx \alpha_e)$	236.9(2)	236.90(4)
$Y_{21} (\approx \gamma_e)$	---	1.17(1)

^aFor comparison with previous LiCl results, our ${}^6\text{Li}{}^{35}\text{Cl}$ measurements were corrected for isotope effects. The atomic masses used were ${}^6\text{Li} = 6.01513$, ${}^7\text{Li} = 7.01601$, ${}^{35}\text{Cl} = 34.96885$, and ${}^{37}\text{Cl} = 36.96590$.

Table VII. Dipole moments for KCl. All values are given in Debyes.

	Dipole Moments	
	Present results	Lee, et al. ²⁷
	$^{39}_{\text{K}}^{35}_{\text{Cl}}$	
μ_0	10.2688(10)	10.48(5)
μ_1	10.3288(15)	
μ_2	10.3877(22)	10.69(5)
	Dipole Moment Functions	
	$\mu_v = \mu_e + \mu_I(v+1/2) + \mu_{II}(v+1/2)^2$	
μ_e	10.2388(12)	
μ_I	0.0610(9)	
μ_{II}	0.0005(4)	
	$^{39}_{\text{K}}^{37}_{\text{Cl}}$	
μ_0	10.2683(22)	

Footnotes and References

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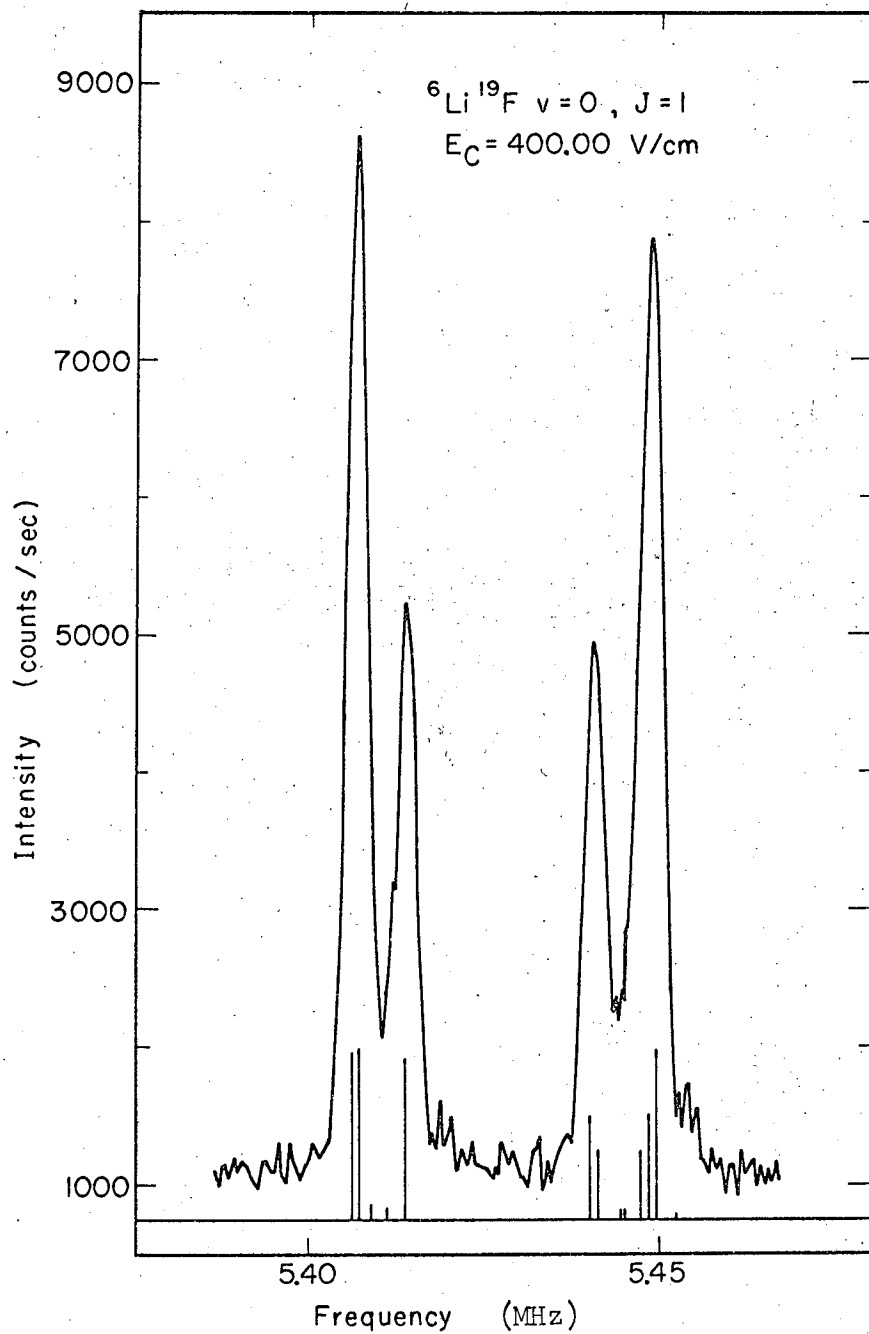
Figure Captions

Fig. 1. A typical spectrum of ${}^6\text{Li}^{19}\text{F}$ with 1.2 kV applied to the deflecting fields. The thin vertical lines represent the calculated spectrum.

FWHM = 3.5 kHz.

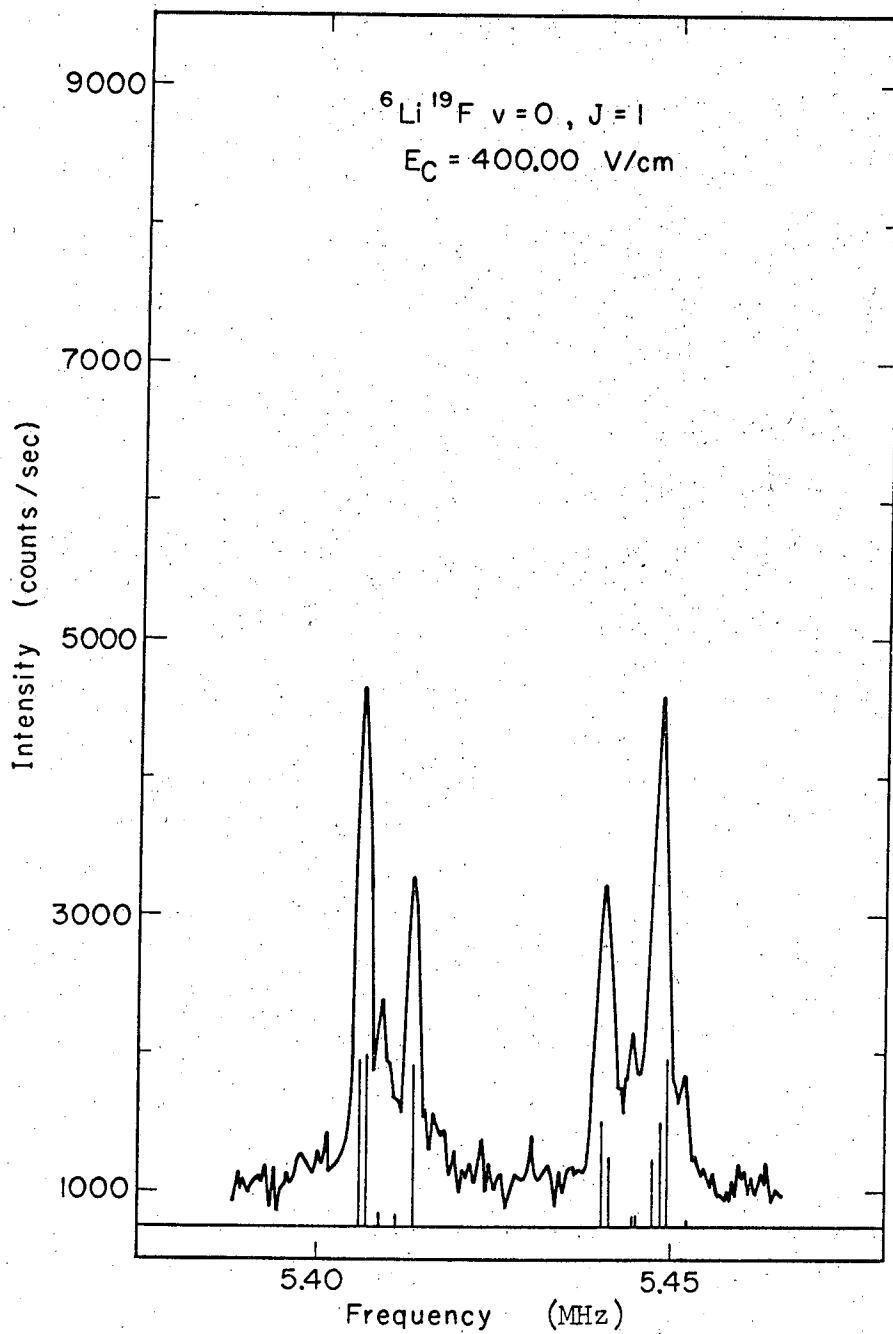
Fig. 2. A typical spectrum of ${}^6\text{Li}^{19}\text{F}$ with 0.6 kV applied to the deflecting fields. The thin vertical lines represent the calculated spectrum.

FWHM = 2.2 kHz.



MUB-3779

Fig. 1.



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Fig. 2.

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