

## Nuclear electric quadrupole moment of ${}^6\text{Li}$

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The molecular beam electric resonance technique has been used to examine the hyperfine spectrum of  ${}^6\text{Li}{}^{19}\text{F}$  for the purpose of obtaining an improved value of the ratio of the electric quadrupole moments of the two lithium nuclei. A total of 29 transitions in vibrational states 0-2 and rotational states 1-4 have been included in a fit to determine the Li nuclear quadrupole interaction along with the magnetic spin-rotation and spin-spin interactions. The magnetic interactions are consistent with values calculated from the previously reported  ${}^7\text{Li}{}^{19}\text{F}$  values, but those have been refitted to take advantage of the new information from  ${}^6\text{Li}{}^{19}\text{F}$ . The electric quadrupole moment ratio of the two lithium isotopes determined from measurements on the two forms of LiF is  $Q({}^6\text{Li})/Q({}^7\text{Li}) = 0.020\,161 \pm 0.000\,013$  (one standard deviation estimate). [S1050-2947(98)08504-7]

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### I. INTRODUCTION

In 1938-9 Kellogg, Ramsey, and Zacharias [1], working in the laboratory of I. I. Rabi at Columbia University, discovered that the molecular beam magnetic resonance spectrum of the deuterated hydrogen molecules could be explained only by including a contribution from an electric quadrupole of the deuterium nucleus. That discovery was particularly significant in that it proved that the nuclear force binding the proton and neutron together in the deuteron was not entirely scalar. Subsequent measurements on other atoms and molecules have yielded values of the nuclear quadrupole moments of most nuclei, stable and unstable, provided the nuclear spin was greater than 1/2. The next simplest nucleus after deuterium with a quadrupole moment is  ${}^6\text{Li}$ . It also has the smallest known quadrupole moment. This paper describes molecular beam electric resonance measurements of the hyperfine spectrum of  ${}^6\text{LiF}$  that yield a significant improvement in the precision of this quantity.

The status of the nuclear quadrupole moments of the first 20 elements has been described by Pyykkö [2]. He notes that

there are in principle several ways by which a nuclear quadrupole moment may be determined:

(1) The nuclear quadrupole coupling constants may be measured in molecules, atoms, or solids. But the constant,  $eQq$ , is a product of two factors: the nuclear moment  $Q$  and the gradient of the electric field at the nuclear site,  $q$ . Thus in order to obtain  $Q$  from these measurements,  $q$  has to be independently calculated or estimated.

(2) The hyperfine spectrum of muonic atoms can be observed. One still needs to separately determine the field gradients to obtain  $Q$ , but this is somewhat simpler than for electronic atoms.

(3) Nuclear scattering using polarized beams can yield information about the multipole moments of the nuclei.

The first method fails in the case of alkali-metal atoms such as lithium, since their S ground states have no field gradient at the nucleus. On the other hand, molecules containing these atoms can be used, for which molecular beam techniques can yield accurate values of  $eQq$ . Urban and Sadlej [3] have calculated  $q$  for the lithium site in LiH, LiF, and LiCl, and, combining this with experimental values for

$eQq$ , have found a value of  $Q = -40.1$  mb for  ${}^7\text{Li}$ . They did not quote an uncertainty, but the values they found varied from  $-39.4$  mb for LiH to  $-40.8$  mb for LiCl. This variation thus corresponds to an uncertainty of 1% or 2% and evidently is due to the limitations of the calculation of  $q$  rather than the experimental uncertainty in  $eQq$ . They also considered the nuclear moment of  ${}^6\text{Li}$ , but in this case their precision was limited by the available experimental values of  $eQq$ .

Method (3), which avoids the problem of calculating molecular wave functions, has been used by Völk and Fick [4] to obtain a value of  $Q = -40.0 \pm 0.6$  mb for the  ${}^7\text{Li}$  nucleus. Their experimental uncertainty by this method is therefore comparable to that in the calculation of  $q$  involved in method (1). They did not attempt a determination for  ${}^6\text{Li}$ .

We have been able to improve the experimental precision of  $eQq$  in  ${}^6\text{LiF}$  so that it now surpasses that of the theoretical value of  $q$ . Since we have experimental values of  $eQq$  for both lithium isotopes in LiF, and  $q$  (as corrected for vibrational and rotational effects) is the same for the lithium site in both, we can circumvent the problem of calculating it by finding the ratio of the two lithium nuclear moments.

In our previously reported study of LiF [5] we found four weak lines, which we attributed to the natural abundance of  ${}^6\text{Li}$  in the sample, and used them to obtain a tentative value of  $eQq$  for  ${}^6\text{LiF}$ . By using an isotopically enriched sample, we have now obtained a much more accurate value of this constant. It turned out that one of the  ${}^6\text{LiF}$  lines observed previously in the natural sample was actually a superposition of the assumed transition with another of a higher vibrational level. This caused a small systematic error in the  ${}^6\text{LiF}$  constants reported. The much stronger signal available with the enriched sample has made it possible to enhance the resolution of our apparatus by decreasing the potential of the electrostatic lenses to select slower molecules from the beam. This has allowed us to resolve these (and other) transitions. We have used a total of 29 transitions involving vibrational states  $v = 0-2$  and rotational states  $J = 1-4$  in a fit to determine the Li nuclear quadrupole interaction as well as the spin-rotation and spin-spin interactions.

## II. DATA

In dealing with diatomic molecules the conventional Hamiltonian [6] is of the form

$$H = H_{\text{elect}} + H_{\text{vib}} + H_{\text{rot}} + H_{\text{hyperfine}} + H_{\text{Stark}}, \quad (1)$$

where

$$\begin{aligned} \frac{H_{\text{hyperfine}}}{h} = & \mathbf{V}_{\text{Li}} \cdot \mathbf{Q}_{\text{Li}} + c_{\text{Li}} \mathbf{I}_{\text{Li}} \cdot \mathbf{J} + c_{\text{F}} \mathbf{I}_{\text{F}} \cdot \mathbf{J} + c_3 \mathbf{I}_{\text{Li}} \cdot \mathbf{D} \cdot \mathbf{I}_{\text{F}} \\ & + c_4 \mathbf{I}_{\text{Li}} \cdot \mathbf{I}_{\text{F}} \end{aligned} \quad (2)$$

and

$$H_{\text{Stark}} = -\boldsymbol{\mu} \cdot \mathbf{E}. \quad (3)$$

Here the first hyperfine term, expressing the lithium nuclear quadrupole interaction, is a scalar product of the rank 2 spherical tensor representing the field gradient at the

nuclear site and that of the nuclear moment itself. There is no such interaction for fluorine because its spin,  $I_{\text{F}}$ , equals 1/2. The second and third terms are the spin-rotation interactions, which arise from the nuclear magnetic moments and the magnetic field due to the rotation of the molecule,  $\mathbf{J}$ . The fourth term is the tensor interaction between the two nuclear magnetic moments and involves the rank 2 tensor  $\mathbf{D}$ . The constant  $c_3$  primarily reflects the ‘‘direct’’ spin-spin effect, which can be calculated from the distance between the nuclei, but also contains a smaller contribution due to the ‘‘electron-coupled’’ interaction. The last term, the scalar spin-spin interaction, is due only to the electron-coupled effect. Each of these terms has its own characteristic effect on the different hyperfine states so that they can be separately evaluated by fitting the experimental spectrum.

The pure hyperfine spectrum of  ${}^6\text{LiF}$  is dominated by the fluorine spin-rotation interaction [the third term in Eq. (2)], so that the appropriate representation to use is the one defined by the coupling

$$\mathbf{F}_1 = \mathbf{J} + \mathbf{I}_{\text{F}}, \quad \mathbf{F} = \mathbf{F}_1 + \mathbf{I}_{\text{Li}}. \quad (4)$$

Standard techniques using the 6- $j$  symbols were used to find the matrices for each of the interaction terms of the Hamiltonian for this representation. The energy levels that result from the fluorine spin-rotation term alone then simplify, within each vibration-rotation state, to

$$\begin{aligned} E = c_{\text{F}} \frac{1}{2} [F_1(F_1 + 1) - J(J + 1) - I_{\text{F}}(I_{\text{F}} + 1)] \\ = c_{\text{F}} \frac{1}{2} \times \begin{cases} J & \text{for } F_1 = J + I_{\text{F}} \\ -(J + 1) & \text{for } F_1 = J - I_{\text{F}} \end{cases} \end{aligned} \quad (5)$$

The separation between these two levels is therefore equal to  $c_{\text{F}}(J + 1/2)$ .

The two levels are each split into three sublevels by the nuclear quadrupole interaction of the  ${}^6\text{Li}$  nucleus, with its spin of 1. The Li spin rotation and the spin-spin interactions produce some further shifts of these levels, but no further splitting. The pure hyperfine spectrum thus consists of a group of lines for each rotational state, centered on the frequency  $c_{\text{F}}(J + 1/2)$ , with a separation within each group of a few kilohertz. The successive vibrational states contribute lines with a similar pattern but shifted by about 1 kHz with each  $v$ , and reduced in size by the Boltzmann factor for the temperature of the oven. This spectrum, with its clear separation of the different rotation states, is simpler and cleaner than the corresponding spectrum of  ${}^7\text{LiF}$ . For that molecule the Li nuclear quadrupole interaction and the  $F$  spin-rotation interaction were of comparable size, so that there was considerable overlap of the lines from different rotational states. For both molecules the electric field could be increased to separate Stark components. This proved to be useful for the positive identification of the lines.

In our molecular beam electric resonance spectrometer, a pair of electrostatic quadrupole lenses is used to focus the beam and as a state selector analyzer. It is the top two levels of the six associated with each rotation-vibration state that are selected, with transitions detectable to the other four states. In addition to the transitions between the two groups

TABLE I. Comparison of experimental data with fit (all frequencies in kHz).

$v$	$J$	$F_1 - F \rightarrow$	$F_1 - F$	Measured	Uncert.	Predicted	Difference	Ratio
0	1	3/2-5/2	1/2-3/2	58.6425	0.0010	58.6438	-0.0013	-1.26
1	1	3/2-5/2	1/2-3/3	57.7576	0.0020	57.7586	-0.0010	-0.49
2	1	3/2-5/2	1/2-3/2	56.869	0.020	56.8970	-0.0280	-1.40
0	1	3/2-5/2	1/2-1/2	52.0190	0.0020	52.0169	0.0021	1.05
1	1	3/2-5/2	1/2-1/2	51.2720	0.0070	51.2591	0.0129	1.85
2	1	3/2-5/2	1/2-1/2	50.544	0.015	50.5183	0.0257	1.71
3	1	3/2-5/2	1/2-1/2	49.830	0.020	49.8108	0.0192	0.96
0	1	3/2-3/2	3/2-1/2	5.067	0.020	5.0765	-0.0095	-0.48
0	1	3/2-3/2	1/2-3/2	57.9510	0.0010	57.9513	-0.0004	-0.35
1	1	3/2-3/2	1/2-3/2	57.0660	0.0030	57.0656	0.0004	0.14
2	1	3/2-3/2	1/2-3/2	56.203	0.020	56.2041	-0.0011	-0.06
0	1	3/2-3/2	1/2-1/2	51.3275	0.0070	51.3245	0.0030	0.43
1	1	3/2-3/2	1/2-1/2	50.580	0.010	50.5661	0.0143	1.43
0	1	3/2-1/2	1/2-3/2	52.8752	0.0020	52.8748	0.0004	0.19
0	2	5/2-7/2	3/2-5/2	95.520	0.010	95.5230	-0.0030	-0.30
1	2	5/2-7/2	3/2-5/2	94.110	0.050	94.0901	0.0199	0.40
2	2	5/2-7/2	3/2-5/2	92.54	0.10	92.6951	-0.1531	-1.53
0	2	5/2-7/2	3/2-3/2	91.5960	0.0050	91.5855	0.0105	2.10
1	2	5/2-7/2	3/2-3/2	90.232	0.015	90.2458	-0.0138	-0.92
2	2	5/2-7/2	3/2-3/2	88.940	0.020	88.9389	0.0011	0.06
0	2	5/2-5/2	5/2-3/2	6.380	0.020	6.3603	0.0197	0.99
0	2	5/2-5/2	3/2-5/2	94.087	0.015	94.0671	0.0199	1.33
0	2	5/2-5/2	3/2-3/2	90.134	0.010	90.1296	0.0044	0.44
1	2	5/2-5/2	3/2-3/2	88.810	0.030	88.7987	0.0113	0.38
0	2	5/2-5/2	3/2-1/2	92.660	0.100	92.6386	0.0204	0.20
1	2	5/2-5/2	3/2-1/2	91.270	0.030	91.2447	0.0253	0.84
0	3	7/2-9/2	5/2-7/2	132.270	0.010	132.2697	0.0003	0.03
0	3	7/2-7/2	7/2-5/2	7.315	0.020	7.3064	0.0086	0.43
0	4	9/2-11/2	7/2-9/2	168.945	0.010	168.9337	0.0113	1.13

of levels, we were able to see some between the sublevels of the top group, at frequencies in the range of 5–8 kHz. All the observed lines are listed in Table I.

The identification and fitting of the observed spectral lines has been made possible by a procedure described previously [7], where a velocity-averaged Rabi line shape is used to deconvolute overlapping transitions. Nevertheless, the same overlap of lines that caused the confusion in interpreting the  ${}^6\text{LiF}$  data in Ref. [5] continued to make it difficult to analyze transitions with  $v > 2$ . The problem is that the vibrational shift in frequency nearly matches the separation due to the Li nuclear quadrupole interaction, so that the (0 1 3/2-3/2  $\rightarrow$  1/2-3/2) line nearly coincides with the (1 1 3/2-5/2  $\rightarrow$  1/2-3/2) line, etc. The weakening of the signal with increasing vibrational state makes the deconvolution procedure less effective.

### III. ANALYSIS

We began the analysis of the spectrum by using the constants from  ${}^7\text{LiF}$  and converting them by the expected factors of moment of inertia and nuclear magnetic and quadrupole moments. This conversion is based on the assumption that the strength of each interaction depends on the internuclear distance in a way that can be represented as a power series in the parameter

$$\xi = (R - R_e)/R_e, \quad (6)$$

following the results derived by Schlier [8]. He showed that any quantity [such as, for example, the field gradient  $q(\xi)$ ] that can be expanded in the series

$$q(\xi) = q_e + q_1\xi + q_2\xi^2 + q_3\xi^3 + q_4\xi^4 \quad (7)$$

will have an expectation value in a given vibrational state  $v$  and rotational state  $J$  that is of the form

$$\begin{aligned} q(v, J) = & (q_e + \alpha B^2) + \beta B(v + 1/2) + \gamma B^2(v + 1/2)^2 \\ & + \delta B^3(v + 1/2)^3 + \epsilon B^2 J(J + 1) \\ & + \eta B^3(v + 1/2)J(J + 1), \end{aligned} \quad (8)$$

where  $\alpha \dots \eta$  are known functions of the  $q_i$  and the Dunham potential coefficients  $a_i$ , and  $B = B_e/\omega_e$  is the ratio of the rotational constant to the vibrational constant. In what follows this expansion will be written in the form

$$q(v, J) = \sum_{i,j} q_{ij}(v + 1/2)^i [J(J + 1)]^j. \quad (9)$$

White [9] showed that the spin-rotation interaction for the  $i$ th nucleus in a molecule should be given approximately by an expression of the form

$$c_i = g_i B_e \frac{4\pi\mu_{0N}}{\hbar} \left[ 4\mu_{0B} \left\langle \frac{1}{r^3} \right\rangle \sum_n \frac{|\langle 0|L|n \rangle|^2}{E_n - E_0} - \frac{q_N}{cR} \right]. \quad (10)$$

In this expression  $g_i$  is the nuclear gyromagnetic ratio,  $B_e$  the equilibrium rotational constant,  $\mu_{0N}$  and  $\mu_{0B}$  the nuclear magneton and Bohr magneton, respectively,  $r$  is the distance from the  $i$ th nucleus to the valence electrons, and the sum is over the states  $n$  of the valence electrons, which are excited by the rotation perturbation. The first term in the brackets gives the effect of the magnetic field produced by these valence electrons on the nucleus in question. The last term represents the effect of the magnetic field produced by the charge  $q_N$  of the other nucleus and its bound electrons, centered at the internuclear distance  $R$ .

If we regard the entire quantity in brackets as a function of the internuclear distance, then this should also be expandable in the same manner as  $q(\xi)$  to give a form similar to Eq. (9), and all we need to do to transform between isotopes is to include the extra dependence on nuclear magnetic moment and the rotational constant. A similar argument should also apply to the spin-spin interactions. This is the justification for our seeking to find experimental values for the coefficients of  $(v+1/2)^i [J(J+1)]^j$  to represent the vibrational and rotational dependence of all the interactions, and also provides the basis for the transformation of the coefficients with isotopic substitution.

With the interaction constants obtained by this procedure, the full Hamiltonian matrix was obtained, within each separate vibrational state, for rotational states  $J = 0$  to 6. This made it possible to include the effects of the matrix elements of the quadrupole interaction which connect states differing by 2 in the rotational quantum number  $J$ . Eigenvalues of this matrix were then found. The line frequencies predicted by this process came close to matching the observed frequencies, but with significant discrepancies. Allowing the  ${}^6\text{Li}$  quadrupole moment to be determined in a fit of the spectrum, as we had intended as a means of more accurately determining the nuclear quadrupole moment ratio for the two lithium isotopes, improved the match, but still left a small but significant discrepancy. Then we realized that the older values of  $B_e$  and  $\omega_e$  that we had been using had been superseded by a more recent investigation and analysis by Maki [10]. When we used these values, the discrepancy dropped to a level consistent with our estimated experimental uncertainty.

There still remained the question of which values of the constants to use. Our lack of  ${}^6\text{LiF}$  data for  $v > 2$  meant that we could not determine the coefficients of  $(v+1/2)^3$  for any of the interactions, but the  ${}^7\text{LiF}$  data did have that information. On the other hand, the fluorine spin-rotation values were more precisely determined by the  ${}^6\text{LiF}$  data. We therefore combined all the measurements from both isotopes into a single fit, incorporating the proper transformations. The  $eQq_{00}$  terms for the two isotopes were fitted separately, but for all others the  ${}^7\text{LiF}$  values were used as the fitted parameters, with the  ${}^6\text{LiF}$  values calculated from them. The reduced chi value of this combined fit was  $\chi = 1.28$ .

TABLE II. Molecular constants determined from fit.

$i, j$	Values refitted from previous ${}^7\text{LiF}$ data		${}^6\text{LiF}$ values calculated from ${}^7\text{LiF}$ values	
Li quadrupole ( $eQq_{ij}$ ):				
0,0	420.810	$\pm 0.029^a$	8.4841	$\pm 0.0052^a$
1,0	-9.898	$\pm 0.077$	-0.2113	$\pm 0.0016$
2,0	0.170	$\pm 0.052$	0.0038	$\pm 0.0012$
3,0	-0.0130	$\pm 0.0097$	-0.00031	$\pm 0.00023$
0,1	0.0030	$\pm 0.0025$	0.000068	$\pm 0.000057$
1,1	-0.0068	$\pm 0.0029$	-0.000163	$\pm 0.000068$
Li spin rotation ( $c_{\text{Li}ij}$ ):				
0,0	1.8935	$\pm 0.0011$	0.80411	$\pm 0.00046$
1,0	-0.0281	$\pm 0.0020$	-0.01265	$\pm 0.00089$
2,0	-0.00036	$\pm 0.00070$	-0.00017	$\pm 0.00033$
0,1	-0.000077	$\pm 0.000055$	-0.000037	$\pm 0.000026$
F spin rotation ( $c_{\text{F}ij}$ ):				
0,0	32.9504	$\pm 0.0043$	36.9547	$\pm 0.0049$
1,0	-0.463	$\pm 0.012$	-0.550	$\pm 0.014$
2,0	-0.0008	$\pm 0.0076$	-0.0010	$\pm 0.0096$
3,0	0.0014	$\pm 0.0013$	0.0018	$\pm 0.0018$
0,1	-0.00160	$\pm 0.00017$	-0.00201	$\pm 0.00021$
1,1	0.00027	$\pm 0.00026$	0.00036	$\pm 0.00035$
Tensor spin-spin ( $c_{3ij}$ ):				
0,0	11.4294	$\pm 0.0036$	4.3279	$\pm 0.0014$
1,0	-0.2128	$\pm 0.0072$	-0.0853	$\pm 0.0029$
2,0	0.0036	$\pm 0.0025$	0.0015	$\pm 0.0010$
0,1	0.00001	$\pm 0.00042$	0.00000	$\pm 0.00018$
Scalar spin-spin ( $c_{4ij}$ ):				
0,0	0.1753	$\pm 0.0018$	0.06638	$\pm 0.00066$
1,0	-0.0055	$\pm 0.0020$	-0.00221	$\pm 0.00081$

<sup>a</sup>Constants determined independently for the two isotopes.

The results are shown in Table II. The uncertainties listed in the table are one standard deviation estimates, which have been adjusted to take into account the reduced chi value of the fit.

To find the nuclear quadrupole moment ratio we have used simply the ratio of the constants  $eQq_{00}$ , which is

$$\frac{{}^6Q}{{}^7Q} = \frac{e^6 Q q_{00}}{e^7 Q q_{00}} = \frac{8.4841 \pm 0.0052 \text{ kHz}}{420.810 \pm 0.029 \text{ kHz}} = 0.020161 \pm 0.000013. \quad (11)$$

In doing this we have neglected the fact that  $q_{00}$  and  $q_e$  are not quite the same. The difference between them is the term  $\alpha B^2$  in Eq. (8). Comparing Schlier's expressions, we note that  $\alpha B^2$  is about an order of magnitude smaller than  $\gamma B^2$ , which is the value of the coefficient of  $(v+1/2)^2$ . According to our fitted value of  $eQq_{20}$ , this should be small in comparison with the uncertainty in  $eQq_{00}$ . It also neglects any contribution to the experimental nuclear quadrupole interaction from a pseudoquadrupole effect. Pyykkö and Linderberg [11] have estimated that the pseudoquadrupole contribution would be less than 0.1 Hz, which is just barely negligible with respect to our experimental uncertainty.

By comparison, the best previous values of this ratio, based on measurements in LiF and LiBr, were 0.0205(20) and 0.0204(10), respectively, as computed by Pyykkö [2] from earlier molecular beam data. Our measurements of  $eQq$  can be combined with Urban and Sadlej's value for the equilibrium field gradient at the Li site in LiF,  $q_e$

$q_e = -0.04415(88)$  a.u., to give  $Q({}^7\text{Li}) = -40.57(81)$  mb and  $Q({}^6\text{Li}) = -0.8178(164)$  mb.

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- [1] J. M. B. Kellogg, I. I. Rabi, N. F. Ramsey, Jr., and J. R. Zacharias, *Phys. Rev.* **55**, 318 (1939).  
[2] P. Pyykkö, *Z. Naturforsch. A* **47**, 189 (1992).  
[3] M. Urban and A. J. Sadlej, *Chem. Phys. Lett.* **173**, 157 (1990).  
[4] H. G. Völk and D. Fick, *Nucl. Phys. A* **530**, 475 (1991).  
[5] J. Cederberg, D. Olson, P. Soulen, K. Urberg, H. Ton, T. Steinbach, B. Mock, K. Jarausch, P. Haertel, and M. Bresnahan, *J. Mol. Spectrosc.* **154**, 43 (1992).  
[6] T. C. English and J. C. Zorn, *J. Chem. Phys.* **47**, 3896 (1967).  
[7] D. Olson, J. Cederberg, P. Soulen, H. Ton, K. Urberg, and B. Mock, *J. Mol. Spectrosc.* **166**, 158 (1994).  
[8] Ch. Schlier, *Fortschr. Phys.* **9**, 455 (1961).  
[9] R. L. White, *Rev. Mod. Phys.* **27**, 276 (1953).  
[10] A. G. Maki, *J. Mol. Spectrosc.* **102**, 361 (1983).  
[11] P. Pyykkö and J. Lindberg, *Chem. Phys. Lett.* **5**, 34 (1970).