

## Letters to the Editor

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### Rotational Magnetic Moments of $\text{Li}^6\text{F}$ and $\text{Li}^7\text{F}^\dagger$

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**T**HE rotational magnetic moments of  $\text{Li}^6\text{F}$  and  $\text{Li}^7\text{F}$  have been measured in a molecular beam electric resonance spectrometer<sup>1</sup> where the conventional electric  $C$  field was replaced with a magnetic field. The results of these measurements are shown in the last row of Table I. These represent the first measurements of the rotational magnetic moment for alkali halide molecules.

Quantum-mechanical expressions for the rotational magnetic moment<sup>2-4</sup> do not lend themselves to numerical evaluation because of the great difficulties involved in obtaining electronic wave functions. However, for diatomic ionic molecules such as the alkali halides an approximation can be made which assumes that the molecule is composed of singly charged ions whose electrons are undisturbed by the presence of the other ion. This ion-pair approximation yields the following expression for the rotational magnetic moment in nuclear magnetons per rotational quantum number:

$$\mu_J/J = (1/m_+) - (1/m_-),$$

where  $m_+$  is the mass of the positive ion in atomic mass units, and  $m_-$  is the mass of the negative ion in atomic mass units. The rotational moments of  $\text{Li}^6\text{F}$  and  $\text{Li}^7\text{F}$  calculated for the ion-pair model are compared with the experimental values in Table I.

The ion-pair approximation neglects the nonslip part of the electronic contribution. This has been calculated by Foley<sup>5</sup> and White.<sup>6</sup> Values based on their results can be used to correct the ion-pair approximation as shown in Table I. The sign of the moment, predicted as positive

TABLE I. Comparison of the predicted and experimental values of  $(\mu_J/J)_{\text{Li}^6\text{F}}$  and  $(\mu_J/J)_{\text{Li}^7\text{F}}$ , in nuclear magnetons per  $J$ .

	$(\mu_J/J)_{\text{Li}^6\text{F}}$	$(\mu_J/J)_{\text{Li}^7\text{F}}$
Ion-pair approximation	+0.114	+0.090
Foley's electronic term	-0.026	-0.023
White's electronic term	-0.040	-0.036
Ion-pair plus Foley's term	+0.088	+0.067
Ion-pair plus White's term	+0.074	+0.054
Experimental values (sign undetermined)	0.0818 $\pm$ 0.0003 $\pm$ 0.0005	0.0642 $\pm$ 0.0002 $\pm$ 0.0004

TABLE II. Rotational magnetic moments of the alkali halides in nuclear magnetons per rotational quantum number as predicted by the ion-pair model.

	$\text{F}^{19}$	$\text{Cl}^{35}$	$\text{Cl}^{37}$	$\text{Br}^{79,81}$	$\text{I}^{127}$
$\text{H}^1$	+0.939	+0.963	+0.965	+0.979	+0.984
$\text{H}^2$	+0.444	+0.468	+0.469	+0.484	+0.488
$\text{H}^3$	+0.279	+0.303	+0.304	+0.319	+0.324
$\text{Li}^6$	+0.114	+0.138	+0.139	+0.154	+0.158
$\text{Li}^7$	+0.090	+0.114	+0.116	+0.130	+0.135
$\text{Na}^{23}$	-0.009	+0.015	+0.016	+0.031	+0.036
$\text{K}^{39}$	-0.027	-0.003	-0.001	+0.013	+0.018
$\text{K}^{41}$	-0.028	-0.004	-0.003	+0.012	+0.016
$\text{Rb}^{85,87}$	-0.041	-0.017	-0.015	-0.001	+0.004
$\text{Cs}^{133}$	-0.045	-0.021	-0.020	-0.005	0.000

by the ion-pair model, was not determined by the experiment.

Table II lists the rotational magnetic moments predicted by the ion-pair model for the alkali halides and the hydrogen halides. The latter are included because of their large ionic character. These values must be considered as an upper bound because they do not include the electronic correction described above. The ion-pair theory predicts that the sign of the moment depends upon the relative masses of the ions. The author wishes to thank Professor John W. Trischka for his help and advice on this work.

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### $M$ -Center Spin Resonance and Oscillator Strength in $\text{LiF}^\dagger$

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**S**OME time ago magnetic resonance data were obtained on a large number of colored  $\text{LiF}$  samples in order to ascertain evidence for  $M$ -center spin resonance. It was established beyond experimental error that the second moment of the spin absorption increased as the strength of x-ray-induced  $M$  optical absorption increased relative to  $F$  absorption. However, it was difficult to estimate quantitatively the separate contributions of  $F$  centers and  $M$  centers until the recent determinations for the  $F$  center alone were made possible by resolved structure measurements.<sup>1</sup> Incorporation of the  $F$ -center results permits a determination of the second moment of the  $M$ -center spin resonance and the ratio of the optical absorption oscillator

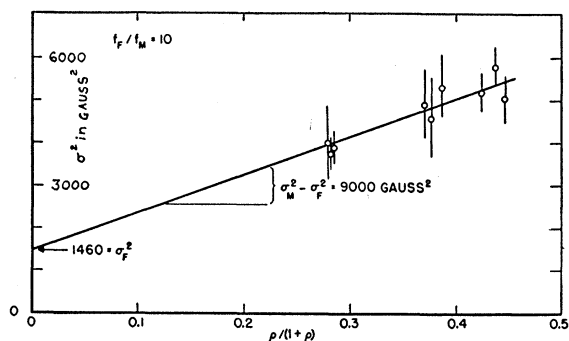


FIG. 1. Variation of the spin resonance second moment,  $\sigma^2$ , with the ratio,  $\rho$ , of  $M$  centers to  $F$  centers.

strengths for the  $M$  and  $F$  centers in their usually recognized bands.<sup>2</sup> Second moment measurements are notoriously lacking in precision and the present report must be considered preliminary.

If we let  $\rho$  be the ratio of the total number of  $M$  centers to  $F$  centers in a given sample and  $\sigma^2$ ,  $\sigma_F^2$ ,  $\sigma_M^2$  be the second moments of the observed and individual spin resonances, we can use the relation

$$\sigma^2 = \sigma_F^2 + \left[ \frac{\rho}{1+\rho} \right] (\sigma_M^2 - \sigma_F^2). \quad (1)$$

It is safe in the samples measured to assume a homogeneous distribution of both types of centers. Then  $\rho$  can be expressed in terms of the measured optical absorption constants  $\mu_M(\nu)$ ,  $\mu_F(\nu)$ , and the unknown oscillator strengths  $f_F$ ,  $f_M$ . The absorption of the  $M$  center is anisotropic<sup>3</sup> and, since unpolarized light was used,  $f_M$  must be considered to be the average over the polarization angle.

$$\rho = (f_F/f_M) \left[ \int \mu_M d\nu / \int \mu_F d\nu \right].$$

It is possible by very prolonged x-ray exposures (up to 2 weeks at room temperature) to vary the second factor from 0.038 to 0.078. The resolved structure measurements provide a point at  $\rho=0$ . This is sufficient to permit a best choice of  $(f_F/f_M)$  which makes the plot of  $\sigma^2$  vs  $\rho/(1+\rho)$  a straight line whose slope is  $(\sigma_M^2 - \sigma_F^2)$ . This plot is shown in Fig. 1 and is drawn for  $f_F/f_M=10$ . Taking  $f_F$  as approximately 0.8,<sup>4</sup> we have 0.08 for  $f_M$ . The value of  $\sigma_M^2$  is around 10 500 gauss<sup>2</sup>. At this stage of the investigation, the probable error in  $f_F/f_M$  can only be guessed at as around 25%. On the other hand,  $\sigma_M^2$  would not change by more than 10% for either limit.

From the only previous theory for the  $M$  center,<sup>5</sup> the magnitude of  $\sigma_M^2$  is reasonable. However, if one carries through the formalism of Inui *et al.* for the coefficients of the LCAO (linear combination of atomic orbitals) in LiF, the results indicate a strongly resolved quartet of equally intense lines. This is in direct con-

tradition to the experimental results obtained which should certainly have revealed this at very high values of  $\rho$ . One expects a lower oscillator strength for the  $M$  center than for the  $F$  center because of the smaller overlap of the excited and ground states. However, it was not expected that the difference would be so large. The investigation is now being continued, using independent methods, to measure the hyperfine interactions and thereby check the determination of  $f_M$ .

I would like to thank Dr. C. K. Jen and Mr. B. S. Gourary for many informative discussions in the course of this work.

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## Double Transitions in the Infrared Spectrum of Solid Hydrogen\*

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IN two previous communications<sup>1,2</sup> the infrared fundamental band of liquid and solid hydrogen at low resolution was described; it has now been recorded with a grating spectrometer and further interpretation of its structure is possible.

Figure 1(a) shows the band in solid normal hydrogen as previously recorded using a prism spectrometer with a spectral slit width of  $15 \text{ cm}^{-1}$ . The three main groups of maxima were correlated with the  $Q$  branch and the  $S(0)$  and  $S(1)$  lines of the collision-induced spectrum of the gas.<sup>1</sup> The broad maxima  $Q_R$ ,  $S_R(0)$ , and  $S_R(1)$  are undoubtedly summation tones of translational lattice frequencies with the molecular vibration and rotation, and correspond to a normal second-order crystal spectrum modified by the free molecular rotation peculiar to solid hydrogen.

The sharp components, on the other hand, are most probably due to induction by the molecular quadrupole moments. Figure 1(b) shows the new detail of the structure obtained using a grating spectrometer with a spectral slit width of  $2 \text{ cm}^{-1}$ . The  $Q$  branch has two components with frequencies near the  $Q(0)$  and  $Q(1)$  Raman frequencies of the solid,<sup>3</sup> and the weak lines designated  $S_1(0)$  and  $S_1(1)$  occur at the calculated positions of the corresponding Raman lines. Each of these lines, therefore, originates in a transition in a