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Letters to the Editor

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Rotational Magnetic Moments of Li^{6}F and Li^{7}F†

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THE rotational magnetic moments of Li^{6}F and Li^{7}F have been measured in a molecular beam electric resonance spectrometer[1] 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[2–4] 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 Li^{6}F and Li^{7}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[5] and White.[6] 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 by the ion-pair model, was not determined by the experiment.

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

	$(\mu_J/J)_{\mathrm{Li^6F}}$	$(\mu_J/J)_{\mathrm{Li^7F}}$
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)	$0.0818_{-0.0003}^{+0.0005}$	$0.0642_{-0.0002}^{+0.0004}$

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

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

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 LiF†

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SOME time ago magnetic resonance data were obtained on a large number of colored 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.[1] 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