

Nuclear Magnetic Moments

S. GOUDSMIT, *University of Michigan*

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This paper contains approximate formulas (Eqs. (5) and (6)) for the calculation of nuclear magnetic moments from observed hyperfine structure separations.

THE hyperfine splitting of an energy level with total angular momentum $Jh/2\pi$ is governed by the formula

$$\delta\nu = AIJ \cos(IJ) \\ = \frac{1}{2}A \{F(F+1) - J(J+1) - I(I+1)\},$$

in which I stands for the nuclear moment in units $h/2\pi$, F is the fine structure quantum number, the resultant of I and J , and the cosine is supposed to be a "quantum" cosine. The proportionality factor A depends in a rather complicated way upon the quantum numbers of the energy state under consideration and is furthermore proportional to the nuclear g -value. In the hyperfine splitting A represents the proportionality factor obtained when one applies the interval rule. It is equal to the distance between two adjacent hyperfine levels divided by the largest of their F values and counted positive when the larger F value belongs to the higher energy.

For a single electron one writes a instead of A and in a hydrogenic case the following formula holds:

$$a = \frac{R\alpha^2 Z^3}{n^3(l+\frac{1}{2})j(j+1)} \frac{g(I)}{1838} \text{ cm}^{-1}. \quad (1)$$

The symbols in this expression have the usual meaning, the nuclear g -value, $g(I)$, is the ratio of the magnetic to the mechanical moment of the nucleus, the former expressed in "proton magnetons" $eh/4\pi Mc$, M being the mass of the proton. In analogy with the electron one expects for a single proton $I = \frac{1}{2}$ and $g(I) = 2$.

For a single outer electron in a penetrating orbit one expects that an approximation similar to that derived by Landé for ordinary multiplet

separations can be applied here. This gives¹:

$$a = \frac{R\alpha^2 Z_i Z_o^2}{n_o^3(l+\frac{1}{2})j(j+1)} \frac{g(I)}{1838} \text{ cm}^{-1}. \quad (2)$$

The derivation of this formula assumes that the properties of the energy state can be considered as arising from two approximately hydrogenic regions of the atom, the outer one with an effective nuclear charge Z_o and a principal quantum number n_o , and the inner one with an average effective nuclear charge Z_i . The value of Z_o is 1 for a neutral atom, 2 for a state of a once ionized atom, etc., n_o is the Rydberg denominator, which can be calculated if the absolute term value is known. The values of Z_i are discussed below.

For non- s electrons the ordinary spin doublets are given by the well-known formula

$$\Delta\nu = \frac{R\alpha^2 Z_i^2 Z_o^2}{n_o^3 l(l+1)} \text{ cm}^{-1}. \quad (3)$$

Combining this with Eq. (2), assuming that Z_i will have the same value in both formulas, one finds

$$a = \frac{\Delta\nu}{Z_i(l+\frac{1}{2})} \frac{l(l+1)}{j(j+1)} \frac{g(I)}{1838} \text{ cm}^{-1}. \quad (4)$$

Earlier applications of these formulas gave unsatisfactory results, the nuclear magnetic moment calculated from the hyperfine structure of different levels of the same atom gave entirely different values. The discrepancy could be explained only in part by the approximate nature of the formulas. Since then it has been shown by

¹ For this formula and the others compare Pauling and Goudsmit, *Structure of Line Spectra*, page 209, reference 1 and page 60.

Breit² and by Racah³ that large relativity corrections must be made to the above formulás. For non-*s* states a corrected equation (4) was used, which indeed seemed to remove the discrepancy between the values of the nuclear magnetic moment obtained from the two levels of the same doublet. For *s* states one did *not* use a corrected equation (2) but used numerically calculated approximate eigenfunctions because the factor in Eq. (2) is proportional to $\psi(0)^2$, the square of the value of the eigenfunction at the origin. The calculations showed that there remained a large discrepancy between the values of the magnetic moment obtained from an *s* state and from other states.

It is a remarkable fact that this discrepancy is much decreased if one uses Eq. (2) with relativity corrections instead of the approximate values of $\psi(0)^2$. Already McLennan, McLay and Crawford⁴ had shown that Eq. (2) is well in agreement with their observations on the hyperfine structure in the spectra of thallium. Furthermore Professor Breit⁵ informed me that the value of $\psi(0)^2$ for the

6*s* state of Cs calculated by Nile by means of a more accurate method than the one used in previous applications comes out to be in very good agreement with Eq. (2). We are thus inclined to believe that the following equations (solved for $g(I)$) are suitable to give fair approximations for the nuclear magnetic moment.

For *s* electrons:

$$g(I) = \frac{3a}{8R\alpha^2} \frac{n_o^3}{Z_i Z_o^2} \frac{1838}{\kappa(\frac{1}{2}, Z_i)}, \tag{5}$$

for non-*s* electrons:

$$g(I) = \frac{aZ_i j(j+1)(l+\frac{1}{2})}{\Delta\nu} \frac{\lambda(l, Z_i)}{l(l+1)} \frac{1838}{\kappa(j, Z_i)}. \tag{6}$$

In these expressions $\kappa(j, Z_i)$ is the relativity correction by which Eq. (2) for the hyperfine structure has to be multiplied, $\lambda(l, Z_i)$ is the same for the multiplet separation Eq. (3). These corrections are given by Eqs. (7) and (8). Table I contains these quantities for $j=\frac{1}{2}$ and $1\frac{1}{2}$ and for $l=1$, for various Z_i values.^{3, 6}

$$\kappa(j, Z_i) = 4j(j+\frac{1}{2})(j+1)/(4\rho^2-1)\rho, \quad \rho^2 = (j+\frac{1}{2})^2 - (\alpha Z_i)^2, \tag{7}$$

$$\lambda(l, Z_i) = [2l(l+1)/(\alpha Z_i)^2] \{ [(l+\frac{1}{2})^2 - (\alpha Z_i)^2]^{\frac{1}{2}} - 1 - [l^2 - (\alpha Z_i)^2]^{\frac{1}{2}} \}. \tag{8}$$

In the application of the above formulas the following remarks are of practical importance. In many-electron spectra the same electron causes often part or all of the hyperfine splitting of several levels. Expressions are known⁷ to obtain the value of *a* for this electron from the various hyperfine structures. If these values turn out to be consistent with each other it may not be considered as a support for the formulas given in the present paper. Only when the values of $g(I)$ calculated from different electrons of the same atom agree can one take this as supporting the validity of the approximations involved.

In a one-electron spectrum the choice of the quantities n_o , Z_o and Z_i is well defined. For *s*-electrons it will be correct to put $Z_i=Z$, the

actual nuclear charge, as the contribution to the interactions comes mainly from the region near the nucleus. For *p*-electrons Z_i as obtained from the doublet formula (3) is throughout the periodic table about equal to $(Z-4)$. It is not

TABLE I.

Z_i	κ		λ $l=1$
	$j=\frac{1}{2}$	$j=1\frac{1}{2}$	
10	1.01	1.00	1.00
20	1.04	1.01	1.00
30	1.09	1.02	1.01
40	1.18	1.03	1.03
50	1.30	1.05	1.05
60	1.49	1.07	1.08
70	1.78	1.10	1.12
80	2.25	1.15	1.17
85	2.61	1.17	1.20
90	3.10	1.20	1.24
92	3.36	1.21	1.27

² Breit, Phys. Rev. **38**, 463 (1931).

³ Racah, Zeits. f. Physik **71**, 431 (1931).

⁴ McLennan, McLay and Crawford, Proc. Roy. Soc. **A133**, 652 (1931).

⁵ Breit, Phys. Rev. **42**, 348 (1932).

⁶ Back-Landé, *Zeemaneffekt und Multiplettstruktur*, page 96.

TABLE II.* Nuclear magnetic moments and g -values.

Z	Element	Atomic weight	I	Magnetic moment	$g(I)$	Remarks
3	Li	7	$1\frac{1}{2}$	3.29	2.19	
13	Al	27	$\frac{1}{2}$	2.1	4.2 B	
29	Cu	63	$1\frac{1}{2}$	2.5	1.7 B	
		65	$1\frac{1}{2}$	2.5	1.7	
31	Ga	69	$1\frac{1}{2}$	2.01	1.34 A	$g(71)/g(69) = 1.27$
		71	$1\frac{1}{2}$	2.55	1.70	
33	As	75	$1\frac{1}{2}$	0.9	0.6 C	
37	Rb	85	$2\frac{1}{2}$	1.3	0.5 C	Rb87 perhaps $I = 2\frac{1}{2}$, magnetic moment 3.0, $g(I) = 1.2$
		87	$1\frac{1}{2}$	2.7	1.8	
48	Cd	111	$\frac{1}{2}$	-0.67	-1.33 B	It is not certain whether 111, 113 or both cause the observed hyperfine structure
		113	$\frac{1}{2}$	-0.67	-1.33	
49	In	115	$4\frac{1}{2}$	5.4	1.2 B	
51	Sb	121	$2\frac{1}{2}$	2.7	1.1 B	$g(121)/g(123) = 1.80$
		123	$3\frac{1}{2}$	2.1	0.6	
80	Hg	199	$\frac{1}{2}$	0.55	1.1 B	$g(199)/g(201) = -2.70$
		201	$1\frac{1}{2}$	-0.62	-0.41	
81	Tl	203	$\frac{1}{2}$	1.8	3.6 A	$g(205)$ about 1% or 2% larger than $g(203)$
		205	$\frac{1}{2}$	1.8	3.6	
82	Pb	207	$\frac{1}{2}$	0.60	1.20 A	
83	Bi	209	$4\frac{1}{2}$	4.0	0.89 A	

* References: Li: reference 9.

Al: Ritschl, Nature **31**, 58 (1933).

Cu: Ritschl, Zeits. f. Physik **79**, 1 (1932).

Ga: Campbell, Nature, in print.

As: Tolansky, Proc. Roy. Soc. **A137**, 541 (1932).

Rb: Kopfermann, Naturwiss. **21**, 24 (1933).

Cd: see Bacher and Goudsmit, *Atomic Energy States*.

In: Jackson, Zeits. f. Physik **80**, 59 (1933).

Sb: Badami, Zeits. f. Physik **79**, 206 and 224 (1932).

Hg, Tl, Pb, Bi, see Bacher and Goudsmit, *Atomic Energy States*.

true that this is the same Z_i as the one occurring in the hyperfine structure formula, the former is the average fourth power, the latter the average third power of the effective nuclear charge. One thus expects for the hyperfine structure Z_i to be somewhat smaller than $(Z-4)$, but how much smaller is quite uncertain. For heavy elements this uncertainty will be within the limit of accuracy of the method employed, but for lighter elements and also for larger l -values, d - and f -orbits, the error will become appreciable, causing the calculated $g(I)$ to be too small.

For a many-electron configuration one must first apply the formulas given in the above-mentioned papers^{6, 7} to derive the a -values for the individual electrons. For non- s electrons

similar formulas exist⁸ which give the $\Delta\nu$ separations for the individual electrons, for p^2 and p^4 for instance, one has to use the total 3P separation. In the case of p^3 , where the multiplet separations are zero in first order, all one can do is to take the 3P separation of the next ion and decrease it slightly to allow for the screening by the third p -electron.

When a single inner s -electron occurs in several configurations it is found that its a -value is practically the same for all of them. This means that there is hardly any screening effect caused by the other electrons. If there is a slight change the largest value of a should be the one where one expects the screening to be least and one may consider this a -value as the one the s -electron has

⁷ Goudsmit and Bacher, Phys. Rev. **34**, 1501 (1929); Goudsmit, Phys. Rev. **37**, 663 (1931).

⁸ Goudsmit, Phys. Rev. **31**, 946 (1928); Humphreys and Goudsmit, Phys. Rev. **31**, 960 (1928); Pauling and Goudsmit, reference 1, p. 157.

in that stage of ionization of the atom in which it is the only outer electron. One should use in Eq. (5) the Z_0 and n_0 for that particular ion. For instance if one obtains a for the 5s electron from the hyperfine structure of the 5s 8s level in neutral cadmium one must use Eq. (5) for once ionized cadmium with this a -value.

More complicated configurations cannot be used in general, unless one is able to obtain some detailed information from the multiplet structure about the coupling scheme of the various angular momentum vectors. The results obtained will not be very reliable.

Table II contains the nuclear magnetic moments and g -values for elements for which the hyperfine structure allows the application of the method described in this paper. The value for

lithium is not obtained by this method, but taken from the very accurate calculations made by Breit and Doermann.⁹ All other results should be considered as preliminary only. In the table the results have been graded A , B , C to denote whether they have been obtained from a few independent hyperfine separations or not. Because of the lack of sufficient data for several elements some personal judgment is needed when Eqs. (5) and (6) have to be applied to a more complicated electron configuration. I consider it therefore better not to discuss in detail the derivations of the results given in Table II, but rather wait for more extensive data to eliminate as much as possible the subjective factor.

⁹ Breit and Doermann, Phys. Rev. **36**, 1732 (1930); Granath, Phys. Rev. **42**, 44 (1932).