Influence of second-order dipole-quadrupole corrections on the octupole hyperfine constant C in ^{133}Cs.

November 20, 2007

Abstract

Recent studies of the influence of second-order dipole-quadrupole interference terms on the the octupole hyperfine constant C in alkaline-earth atoms lead us to re-examine the influence of second-order corrections on hyperfine constant C in ^{133}Cs. We find that the second-order dipole-quadrupole interference terms reduce the value of C in ^{133}Cs by 0.12 Hz; far below the experimental uncertainty of 74 Hz.

Analysis

The first-order contribution to the hyperfine energy for an atomic state with angular momentum J is

$$W_F^{(2)} = \sum_k (-1)^{I+J+F} \left\{ \begin{array}{ccc} I & J & F \\ J & I & k \end{array} \right\} \langle I \| T_k^{(n)} \| I \rangle \langle J \| T_k^{(e)} \| J \rangle \qquad (1)$$

Introducing the coefficient

$$M(I,J,F,k) = \frac{(-1)^{I+J+F} \left\{ \begin{array}{ccc} I & J & F \\ J & I & k \end{array} \right\}}{\left(\begin{array}{ccc} I & k & I \\ -I & 0 & I \end{array} \right) \left(\begin{array}{ccc} J & k & J \\ -J & 0 & J \end{array} \right)}, \qquad (2)$$

The first-order coefficient can be written in terms of stretched matrix elements as

$$W_F^{(2)} = \sum_k M(I,J,F,k) \langle II | T_k^{(n)} | II \rangle \langle JJ | T_1^{(e)} | JJ \rangle. \qquad (3)$$

These stretched matrix elements, in turn, serve to define the $(A, B, C, \cdots)$ hyperfine constants

$$\begin{aligned}
A &= \frac{1}{IJ}\,\langle II|T_1^{(n)}|II\rangle\langle JJ|T_1^{(e)}|JJ\rangle = \frac{\mu_I}{IJ}\,\langle JJ|T_1^{(e)}|JJ\rangle && (4)\\
B &= 4\,\langle II|T_2^{(n)}|II\rangle\langle JJ|T_2^{(e)}|JJ\rangle = 2Q\,\langle JJ|T_2^{(e)}|JJ\rangle && (5)\\
C &= \langle II|T_3^{(n)}|II\rangle\langle JJ|T_3^{(e)}|JJ\rangle = -\Omega\,\langle JJ|T_3^{(e)}|JJ\rangle && (6)\\
D &= \langle II|T_4^{(n)}|II\rangle\langle JJ|T_4^{(e)}|JJ\rangle = \Pi\,\langle JJ|T_4^{(e)}|JJ\rangle && (7)
\end{aligned}$$

The second-order contribution to the hyperfine energy of a state F from a nearby fine-structure state with angular momentum J' is

$$W_F^{(2)} = \left\{\begin{array}{ccc} I & J & F \\ J' & I & 1 \end{array}\right\}^2 \frac{\left|\langle I\|T_1^{(n)}\|I\rangle\right|^2 \left|\langle J\|T_1^{(e)}\|J'\rangle\right|^2}{E_J - E_{J'}}$$
$$+2\left\{\begin{array}{ccc} I & J & F \\ J' & I & 1 \end{array}\right\}\left\{\begin{array}{ccc} I & J & F \\ J' & I & 2 \end{array}\right\} \frac{\langle I\|T_1^{(n)}\|I\rangle\langle I\|T_2^{(n)}\|I\rangle\langle J\|T_1^{(e)}\|J'\rangle\langle J\|T_2^{(e)}\|J'\rangle}{E_J - E_{J'}} \qquad (8)$$

Let us write Eq. (8) in the form

$$W_F^{(2)} = \left\{\begin{array}{ccc} I & J & F \\ J' & I & 1 \end{array}\right\}^2 \eta + \left\{\begin{array}{ccc} I & J & F \\ J' & I & 1 \end{array}\right\}\left\{\begin{array}{ccc} I & J & F \\ J' & I & 2 \end{array}\right\}\zeta, \qquad (9)$$

where

$$\begin{aligned}
\eta &= \frac{\left|\langle I\|T_1^{(n)}\|I\rangle\right|^2 \left|\langle J\|T_1^{(e)}\|J'\rangle\right|^2}{E_J - E_{J'}} && (10)\\
\zeta &= 2\frac{\langle I\|T_1^{(n)}\|I\rangle\langle I\|T_2^{(n)}\|I\rangle\langle J\|T_1^{(e)}\|J'\rangle\langle J\|T_2^{(e)}\|J'\rangle}{E_J - E_{J'}}. && (11)
\end{aligned}$$

For the $7p_{3/2}$ state of ^{133}Cs (I=7/2) where J'=1/2, we find that the energies are given in terms of the hyperfine constants by

$$\begin{aligned}
W_2 &= -\frac{27}{4}A + \frac{15}{28}B - \frac{33}{7}C && (12)\\
W_3 &= -\frac{15}{4}A - \frac{5}{28}B + \frac{55}{7}C - \frac{1}{56}\zeta + \frac{1}{56}\eta && (13)\\
W_4 &= \frac{1}{4}A - \frac{13}{28}B - \frac{33}{7}C + \frac{1}{72}\zeta + \frac{5}{216}\eta && (14)\\
W_5 &= \frac{21}{4}A + \frac{1}{4}B + C && (15)
\end{aligned}$$

We rewrite these equations in terms of energy differences $\delta W_k = W_k - W_{k+1}$ and solve for the (A, B, C) hyperfine constants.

$$\begin{aligned}
A &= -\frac{3}{56}\delta W_2 - \frac{2}{21}\delta W_3 - \frac{11}{120}\delta W_4 - \frac{\zeta}{1260} + \frac{\eta}{1512}\\
B &= \frac{5}{8}\delta W_2 + \frac{1}{3}\delta W_3 - \frac{77}{120}\delta W_4 + \frac{\zeta}{120} + \frac{\eta}{36}\\
C &= -\frac{1}{32}\delta W_2 + \frac{1}{24}\delta W_3 - \frac{7}{480}\delta W_4 + \frac{\zeta}{480} && (16)
\end{aligned}$$

Table 1: Reduced dipole and quadrupole matrix elements (MHz) and A & B hyperfine constants (MHz) for $6p$ states in ^{133}Cs. (μ_I=2.5826, Q= -3.43(mb), I=5/2)

$A(6p_{1/2})$	$A(6p_{3/2})$	$\langle 6p_{3/2} \| T_1 \| 6p_{1/2} \rangle$	$B(6p_{3/2})$	$\langle 6p_{3/2} \| T_2 \| 6p_{1/2} \rangle$
290.26	51.09	22.52	-0.4864	349.78
291.89(6)	50.288		-0.4940(17)	

Evaluation of the second-order corrections

We can write the second-order corrections as

$$\eta = \frac{(I+1)(2I+1)}{I} \mu_I^2 \frac{\left| \langle J \| T_1^{(e)} \| J-1 \rangle \right|^2}{E_J - E_{J'}} = \frac{72}{7} \mu_I^2 \frac{\left| \langle J \| T_1^{(e)} \| J-1 \rangle \right|^2}{E_J - E_{J'}} \tag{17}$$

$$\zeta = \frac{(I+1)(2I+1)}{I} \sqrt{\frac{2I+3}{2I-1}} \mu_I Q \frac{\langle J \| T_1^{(e)} \| J-1 \rangle \langle J \| T_2^{(e)} \| J-1 \rangle}{E_J - E_{J'}} = \frac{72}{7} \sqrt{\frac{5}{3}} \mu_I Q \frac{\langle J \| T_1^{(e)} \| J-1 \rangle \langle J \| T_2^{(e)} \| J-1 \rangle}{E_J - E_{J'}} \tag{18}$$

We do a second-order MBPT calculation of the matrix elements in the above formulas and show the results in Table 1. Based on the comparison of the theoretical hyperfine constants with experiment, we expect the error in the off-diagonal matrix elements to below 2%.

Combining data, as done in the attached spread-sheet, leads to the conclusion that the second-order dipole-quadrupole interference term reduces the the lowest-order value of the octupole constant C by 0.12 Hz. The experimental hyperfine frequencies are taken from [1]. The present analysis of η agrees with that given in [2]. The value of Q used in the evaluation of ζ is taken from [3]. The resulting values of the hyperfine constants are

$$A = 50.28825(23)$$
$$B = -0.4940(17)$$
$$C = 0.00056(7).$$

References

[1] V. Gerginov, A. Derevianko, and C. E. Tanner, Phys. Rev. Lett. **91**, 072501 (2003).

[2] W. R. Johnson, H. C. Ho, C. E. Tanner, and A. Derevianko, Phys. Rev. A **70**, 014501 (2004).

[3] M. Pernpointner, P. Schwerdtfeger, and B. A. Hess, J. Chem Phys. **108**, 6739 (1998), The nuclear quadrupole moment (NQM) of the 133 isotope of Cs is not accurately known. This is due to the fact that the electric field gradient (EFG) of Cs for the 6p1 2P3/2 excited state was only estimated from the 6pr3 expectation value using HartreeSlater calculations. CsF microwave data yield a very accurate nuclear quadrupole coupling constant (NQCC). We therefore decided to perform relativistic coupled cluster calculations for CsF in order to obtain a more accurate value for the Cs EFG. At the highest level of theory we obtain a NQM for the first vibrational-rotational state of 3.43(10) mb which should be more accurate than the previously estimated value of 3.7(1.6) mb or 9(4) mb.

Analysis of Cs Hyperfine Constants
11/20/2007

Experimental data: Wk = Exp[k]-Exp[k+1] MHz

W4	-251.09160
W3	-201.28710
W2	-151.22470

Experimental Uncertainties MHz

dW4	0.00200
dW3	0.00110
dW2	0.00160

Lowest-Order Calculation

A0(MHz)	50.28825
B0(MHz)	-0.49403
C0(MHz)	0.00056

Second-Order Correction

Q(b)	-0.00343
mu	2.58260
I	3.50000
Eden (MHz)	1.6610E+07
T1(MHz)	22.52033
T2(MHz)	349.77600
eta(MHz)	0.00209
zeta(MHz)	-0.00006

Second-Order Additions

A2	1.4297E-06
B2	5.7723E-05
C2	-1.1622E-07

Estimated 4% error

dA2	5.7188E-08
dB2	2.3089E-06
dC2	-4.6487E-09

Final value for A,B,C

A0+A2(MHz)	50.28825
B0+B2(MHz)	-0.49397
C0+C2(MHz)	0.00056

Combine expt and theor uncertainties

dA	0.00023
dB	0.00167
dC	0.00007

Summary: Including Dipole-Quadrupole corrections decreases value of C by 0.12 Hz