

Measurements of hyperfine constants in Ca^+

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We have measured the hyperfine constants $A(^2S_{1/2})$, $A(^2P_{1/2})$, and $A(^2P_{3/2})$ for Ca^+ . We compare our results with the calculations of Mårtensson-Pendrill and Salomonson [Phys. Rev. A **30**, 712 (1984)], who used many-body perturbation theory (MBPT). The agreement between our results and MBPT calculations for Ca^+ is about 3%, which is comparable to similar comparisons reported for Cs [S. Blundell, in *Relativistic, Quantum Electrodynamical, and Weak Interaction Effects in Atoms*, AIP Conf. Proc. No. 189, edited by Walter Johnson, Peter Mohr, and Joseph Sucher (AIP, New York, 1988)].

Recent investigation of parity nonconservation (PNC) in atomic systems have shown that theoretical precision of 1% or less is necessary for meaningful comparison with experiment, as pointed out by Blundell.¹ While heavier atoms are better suited for the experimental studies of PNC, theoretical calculations for these atoms are lengthy and require extensive numerical calculations using supercomputers. It is therefore desirable to test the success of these calculations, in terms of both their rate of convergence and level of precision, in simpler systems before undertaking the more extensive PNC calculations. Any PNC effects are, of course, particularly sensitive to the wave function in or near the nucleus; so other quantities that depend upon $|\Psi(0)|^2$ are of particular interest. Two of these are the field-effect portion of the isotope shift and the hyperfine splitting constants. We have been studying both of these for the resonance lines of Ca^+ . By now we have determined the hyperfine splitting constants $A(^2S_{1/2})$, $A(^2P_{1/2})$, and $A(^2P_{3/2})$ for ^{43}Ca with good precision, and this paper presents these results for comparison with any theoretical work such as that of Mårtensson-Pendrill and Salomonson.² Soon we hope also to publish measurements of the isotope shifts for these resonance lines, and for all stable isotopes of calcium.

Prior to this work there was available only the value for $A(^2S_{1/2})$ reported by Kelly, Kuhn, and Pery.³ We believe that our results have considerably greater precision than that as well as that they give the hyperfine splitting constants for the two excited states. Even though our results have larger uncertainties than other measurements used for similar comparison in the alkali-metal atoms,⁴ they still include good enough precision for fine tuning theoretical calculations.

Our experimental setup is basically the same as that reported earlier.⁵ In this experiment we used aluminum cathodes with neon as the carrier gas. The typical operating discharge conditions for an optimal signal consisted of neon pressures of about 1 torr and discharge currents of about 30 mA at 220–250 V dc. We used two different étalon spacers, which have free spectral ranges of 7.495 and 9.293 GHz, respectively. The isotopically enriched samples of calcium purchased from Oak Ridge National Laboratory came in the form of calcium carbonate. The ^{40}Ca was enriched to 99.976 at. % purity.

The ^{43}Ca sample contained 12.46, 0.55, 83.58, and 3.35 at. % of calcium isotopes of mass 40, 42, 43, and 44, respectively. For ease of working with small quantities of the samples (less than 0.5 mg of calcium) we converted each carbonate sample to an aqueous chloride solution, which was poured into the hollow of each individual cathode. The cathodes were then heated to evaporate the water.

A typical run consisted of simultaneous scans through six or seven orders of the ^{43}Ca and ^{40}Ca profiles for either the $4s\ ^2S_{1/2}-4p\ ^2P_{1/2}$ or the $4s\ ^2S_{1/2}-4p\ ^2P_{3/2}$ transitions. For each run the ^{40}Ca scan was used to normalize the scan rate, and thus assign the scale to the energy axis. An "experimental profile" for one order was calculated by suitably combining the several orders. A "theoretical profile" composed of a suitably shaped and positioned Voigt function was then fitted to the experimental profile to provide a low sum of squares of differences for 160 (or 200) sample points in each of the two profiles. The adjustable parameters were the Gaussian and Lorentzian half-widths and the location of the center of the Voigt function in the profile. For ^{40}Ca a single Voigt function was sufficient and its center provided a reference point for the ^{40}Ca impurity contribution in the ^{43}Ca profile of that run. The ^{43}Ca theoretical profile required separate Voigt functions for each hyperfine component and for each even isotope impurity. The locations of the centers of the Voigt functions for the impurities relative to ^{40}Ca were taken to be constant values based on our previous isotope shift runs (for ^{40}Ca to ^{42}Ca , 434.7 MHz, ^{40}Ca to ^{44}Ca , 860.4 MHz). The adjustable parameters then became the Gaussian and Lorentzian half-widths (each taken to be the same for all components), $A(^2S_{1/2})$, $A(^2P)$, and the center of the hyperfine pattern relative to that of ^{40}Ca . Any contribution due to the electric quadrupole term, $B(^2P_{3/2})$, was considered to be negligible, because of the small value of the nuclear electric quadrupole moment,⁶ and was not taken into account in the fit.

In all the runs we obtained Lorentzian and Gaussian half-widths of about 600 and 1200 MHz, respectively. Generally, an increase in the discharge current or pressure resulted in an increase in the Gaussian half-width, but other fitted parameters, including $A(S)$ and $A(P)$, remained insensitive to the discharge conditions. Table I shows the values of the hyperfine splitting constants for

TABLE I. Hyperfine splitting constants for Ca^+ (MHz). Numbers in parentheses represent one standard deviation.

	Present Experiment	Ref. 2	Ref. 3
$A(4s\ ^2S_{1/2})$	-797.5(2.4)	-819	-817
$A(4p\ ^2P_{1/2})$	-158.0(3.3)	-148	
$A(4p\ ^2P_{3/2})$	-29.7(1.6)	-30.9	

Ca^+ . The first column is the results of the present experiment for which the numbers in parentheses represent one standard deviation; the second column is the calculated values of Mårtensson-Pendrill and Salomonson;² and the third column is the measured results of Kelly, Kuhn and Pery.³ Our results for the value of $A(^2S_{1/2})$ are based on the average of 38 runs, 16 of which involve the analysis of the profile for the transition from the $^2P_{1/2}$ and the rest for the transition from the $^2P_{3/2}$ state. Only five of these runs resulted in values that were two or three standard deviations from the average; also, all the variations were independent of the particular transition. The consistency of the values of $A(^2P_{1/2})$ and $A(^2P_{3/2})$ was even better.

Our choice of one standard deviation for the uncertainty is based upon the remarkable consistency of our results even with changes of discharge conditions and use of different spacers. In our isotope shift experiment, étalon misalignment from parallelism is probably the primary source of systematic errors. To check for the effect of étalon misalignment we performed several sets of trial runs. In one trial set we used natural calcium in both cathodes and measured the "zero isotope shift." This shift was no larger than 3 MHz. In a similar test, immediately after completing a ^{40}Ca - ^{43}Ca run, we measured the zero isotope shift for a neighboring aluminum line. These runs also resulted in zero shifts of 3 MHz or less. Since we only used the results of our isotope-shift measurements to correct for the impurities in our ^{43}Ca sample, any uncertainty introduced by étalon misalignment should be negligible for the results reported in this paper, and it is likely that the variations from run to run are entirely due to the noise and the width of the profile. All in

all, based on the consistency of our results from run to run, and in the absence of other experimental procedures, we feel that one standard deviation, as quoted, is a reasonable estimate of the uncertainties in our results.

Kelly, Kuhn and Pery,³ by cooling their cathodes in a liquid-hydrogen bath, resolved the hyperfine structure and took long exposures recorded on a photographic plate to determine the ground-state splitting to be $W=109\pm 2$ mK. If we take the precision of the hyperfine splitting constant $A(^2S_{1/2})$ derived from W to be about 1 mK, then their result of $A(^2S_{1/2})=810\pm 30$ MHz will be in agreement with our measured value.

The agreement between our results and those calculated by Mårtensson-Pendrill and Salomonson² is as good as a similar comparison for ^{39}K reported by Johnson, Idrees, and Sapirstein.⁴ In both of these comparisons theory and experiment agree best in the value of $A(^2S_{1/2})$ and disagree most in the value of $A(^2P_{1/2})$. However, while the measured ground-state hyperfine constant is larger than the calculated value for K, for Ca^+ the measured value is smaller.

In their calculation Mårtensson-Pendrill and Salomonson² found that use of relativistic Dirac-Fock orbitals instead of nonrelativistic Hartree-Fock orbitals resulted in a 4.4% increase of both the first-order $\langle r^{-3} \rangle$ and the core-polarization contributions. Based on this, they estimated a 4.4% increase in the absolute value of the hyperfine splitting constants. This estimate causes the value of the splitting constants $A(^2S_{1/2})$ and $A(^2P_{3/2})$ to move further from our results, but gives a closer agreement for the $A(^2P_{1/2})$ value. It appears that a more complete relativistic treatment is required to determine whether inclusion of such effects is necessary for better agreement between theory and experiment.

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¹S. Blundell, in *Relativistic, Quantum Electrodynamics, and Weak Interaction Effects in Atoms*, Proceedings of the Program held on Relativistic, Quantum Electrodynamics, and Weak Interaction Effects in Atoms at the Institute of Theoretical Physics, Santa Barbara, CA, 1988, AIP Conf. Proc. No. 189, edited by Walter Johnson, Peter Mohr and Joseph Sucher (AIP, New York, 1988).

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