Isotope-shift measurements in Ca^+

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We have measured the optical shifts for all stable isotopes of Ca^+, with respect to isotope mass 40, in the resonance transitions $4s\,^2S_{1/2}-4p\,^2P_{1/2,3/2}$. The value of our measured shift for the even isotope mass 46 falls below the King plot. From the fit to a second King plot, omitting the shift for mass 46, we obtain a value of -312 MHz fm^{-2} for the field-shift constant F. A comparison of this value with *ab initio* calculations [G. Torbohm, B. Fricke, and A. Rosen, Phys. Rev. A **31**, 2038 (1985)] and our semiempirical estimate shows better agreement when correlation effects have been included in the calculations [A.-M. Martensson-Pendrill, A. Ynnerman, and H. Warston (private communication)] and suggests that inclusion of the screening factor β in semiempirical methods results in an overestimate of F.

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Optical isotope-shift measurements have traditionally complemented electron scattering and muonic x-ray data for determining values of the nuclear charge parameter $\delta\langle r^2\rangle$, the change in the mean-square charge radius due to addition of neutrons [1]. In this process one also makes a determination of the difference between the values of the electronic density at the nucleus of the initial and final states, $\Delta|\Psi(0)|^2$. Similarly, measured values of the hyperfine splitting constants, A, when put into an appropriate theoretical formulation [1] give a measure of $|\Psi(0)|^2$. A comparison of the values obtained both ways helps check the validity of the formula for A and additionally provides an experimental value of $|\Psi(0)|^2$ to compare with *ab initio* theoretical calculated values.

Recent high-precision Doppler-free laser experiments [2–4] and extensive analysis of all experimental data [5] for the case of neutral Ca have led to very accurate determination of $\delta\langle r^2\rangle$ for all stable isotopes. But because of configuration interaction, one cannot be sure of the theoretical predictions. A more suitable case for such a comparison is the alkalilike Ca^+, for which recent theoretical calculations by Martensson-Pendrill and Salomonson [6] of the hyperfine splitting constants, also very sensitive to the electron's wave function near the origin, have produced excellent agreement with measurements and have now been extended to the calculation of the field-shift constant [7]. Also, the optical isotope-shift measurements for Ca^+ can be combined with the already accurately determined values of $\delta\langle r^2\rangle$ for Ca to provide more reliable values of the mass- and field-shift constants than could be determined from the shift measurements alone. The experiments reported in this paper were undertaken with this in mind.

Our experimental setup and analysis of the data are basically the same as in our previous work [8] on the measurement of the hyperfine constants in Ca^+. In the case of the even isotope samples for mass 42, 44, and 48 the only significant contribution to the experimental profile due to an impurity was that due to the presence of mass 40 in the sample, as shown in Table I. Our theoretical profile which was fitted to the experimental profile was thus made of two Voigt functions which were scaled to the relative amount of the two isotopes present in the sample. The center of the Voigt function representing the profile for mass 40 was assigned the value obtained from the fit to the superposed experimental profile of the signal from the cathode containing mass 40 for the same run. A similar procedure was used in the fittings of the profiles for mass 46, except that for these fits two additional Voigt functions (one for the contribution of mass 44 and another for mass 48) were included in the theoretical profile. The centers of these two functions were shifted, with respect to the Voigt function for mass 40, by the averaged isotope-shift values measured for those masses

TABLE I. Enrichment of isotope samples (purchased from Oak Ridge National Laboratory) used in this experiment.

	Samples used					
Isotope present in the sample	^{40}Ca	^{42}Ca	^{43}Ca	^{44}Ca	^{46}Ca	^{48}Ca
40	99.976	5.45	12.46	1.363	62.23	2.20
42	0.005	94.10	0.55	0.038	0.72	0.03
43	0.001	0.61	83.58	0.026	0.18	<0.01
44	0.017	0.38	3.35	98.57	4.46	0.07
46	<0.001	<0.001	<0.001	<0.005	30.73	<0.005
48	<0.001	<0.01	0.06	0.007	1.68	97.69

TABLE II. Measured isotope shifts. All shifts are given with respect to mass 40, in units of MHz. The numbers in parentheses represent one standard deviation.

Isotope mass	Present work	Ref. [10]	Ref. [9]	Ref. [11]
42	436.2(22.8)	401±3		468
43	684.7(36.3)			
44	839.4(14.7)			
46	1256.7(35.7)			
48	1758.0(24.0)		1798.7±60	

in preceding runs. Similar to the case of mass 40 isotope the three adjustable parameters of the fits for all of the even mass runs were Gaussian and Lorentzian half-widths, taken to be the same for all isotope contributions to that sample, and the center of Voigt function representing the profile for that isotope.

Table II gives the values of our measured shifts, as well as other published results. Our measured shifts for the two transitions $4s\ ^2S_{1/2}-4p\ ^2P_{1/2,3/2}$ were equal, for all isotope pairs, within our experimental uncertainties. Thus the values reported in Table II are the average of the runs including both of these transitions. These averages are over 36, 45, 27, 13, and 26 runs for mass 42, 43, 44, 46, and 48 measurements, respectively. The uncertainties quoted in Table II each represent one standard deviation. Of the 147 runs, most resulted in shifts which differed from the average by less than one standard deviation and only five runs gave values two or three standard deviations away from the average. As in the case with our hyperfine measurement reported earlier [8] we believe that most of the variations from run to run are due to discharge instabilities, a problem which, in retrospect, could perhaps be minimized by using larger amounts of enriched isotopes in the cathodes. The larger standard deviations in the shifts for isotopes mass 43 and 46 are most likely due to the relatively low intensities of the discharges, since the cathodes for these runs did not contain more than 0.5 mg of the enriched isotopes.

The agreement between our results and those of Pery [9], who used photographic detection with long exposures and a 75%-enriched sample of mass 48, is strikingly good. Our results for the shift between mass 40 and 42, however, does not agree well with those reported by Bruch *et al.* [10,11]. Unfortunately, there is little information in either of these two published reports about the details of the experiment to allow us to say more about this comparison, except that our measured shift seems to fall between the two values that they have reported.

We have used the values of our isotope shifts listed in Table II along with those of Palmer *et al.* (from Table I of Ref. [5]) in a King plot and taking their values of $\delta\langle r^2\rangle$ gives the values of field- and mass-shift constants $F=-268(77)$ MHz fm^{-2} and $M=409.0(8.2)$ GHz u, respectively (the numbers in the parentheses represent the standard error of the fit). Using the semiempirical relation, Eq. 4.28 of King [12], with $\mu_i=-1.317\,642\ \mu_N$ as given by Olsson and Salomonson [13] and $A_s=-797.5$ MHz from Ref. [8] we obtain for the field-shift constant a value of -293.2 MHz fm^{-2}, without inclusion of screening effects. Inclusion of the relativistic screening factor of $\beta=1.114$ of Ref. [14] increases the value of F to -326.6 MHz fm^2. Using the relativistic single-configuration Dirac-Fock wave functions Torbohm, Fricke, and Rosen [14] calculate $\Delta|\Psi(0)|^2$ and quote a result of -249.2 MHz fm^{-2} for F. Martensson-Pendrill, Ynnerman, and Warston [7] use many-body perturbation calculations including relativistic corrections and correlation effects to get $F=-285(3)$ MHz fm^{-2}. The result of the field-shift constant F, using all of our measured shifts, seems to fall between the two *ab initio* calculations [14,7] and far below the semiempirical result. This is primarily because our measured shift for mass 40–46 falls below the King plot. The value of this shift is based on fewer runs. Also, the relatively low intensity of the signal as well as the poor enrichment of the sample could account for this discrepancy in the King plot. We have made a second King plot which does not include the effect of mass 46 data. From this plot we get values of $F=-312(46)$ MHz fm^{-2} and $M=417.6(5.3)$ GHz u. This value of F agrees best with the *ab initio* calculations of Martensson-Pendrill, Ynnerman, and Warston [7] and suggests the importance of correlation effects, which tend

TABLE III. Comparison of the field-shift constant F (MHz fm^{-2}).

F	Reference
$-268(77)$	present work, full King plot
$-312(46)$	present work, King plot excluding mass 46 data
-293	semiempirical, using A_s of Ref. [8], and $\beta=1$
-326.6	semiempirical, using A_s of Ref. [8], and $\beta=1.114$
$-285(3)$	*ab initio* calculation, Ref. [7]
-249.2	*ab initio* calculation, Ref. [14]

to increase the calculated value of F. We have summarized these comparisons in Table III.

In a similar work for potassium, Martensson-Pendrill, Pendrill, Salomonson, Ynnerman, and Warston [15] calculated a value of F about 14% smaller than the value obtained from the experimental data using a semiempirical estimate including the screening factor—very similar to the 13% difference in the present comparison. In the case of Ca^+ the agreement between the theory and experiment for A_s is excellent, which suggests that the values of the screening factors, β, used in the semiempirical estimates result in overestimating the field-shift constants derived from the optical shift measurements. This is in general agreement with the conclusion reached by Torbohm, Fricke, and Rosen [14] but suggests a smaller discrepancy. Of course, it is always ideal to compare experimental results with calculations based directly on the theory. However, in the light of the extensive work required in *ab initio* calculations, an improvement of the values of screening factors could alternatively serve to render these simple estimates rather useful.

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