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Isotope shift of the 2s $^2S_{1/2} \rightarrow$ 2p $^2P_{1/2,3/2}$ transitions of Li-like Ca ions*

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The mass- and field-shift parameters of the two 2s $^2S_{1/2} \rightarrow$ 2p $^2P_{1/2,3/2}$ transitions in the Li-like Ca ions are calculated by using multi-configuration Dirac–Hartree–Fock (MCDHF) and the relativistic configuration interaction (RCI) methods with the inclusion of the transverse photon (Breit) interaction, vacuum polarization and self-energy corrections. In addition, the mass shift and field shift of these two transitions are calculated, where the field shift is calculated by using the evaluated value $\delta\langle r^2\rangle$ obtained by [*Atomic Data and Nuclear Data Tables* **99** 69 (2013)]. It is found that the mass shift of Li-like Ca ions is greater than the field shift.

Keywords: isotope shift, multi-configuration Dirac–Hartree–Fock (MCDHF), mass shift, field shift

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1. Introduction

Isotopes have different mass and charge distributions, which lead to the difference on the physical observable quantities. The energy or wavelength shifts of the specific transition line in the spectrum from different isotopes which were known as isotope shift (IS), mainly come from two contributions: the mass shift (MS) and the field shift (FS). The MS is due to the finite mass of the nucleus, whereas the FS is caused by the difference in the nuclear charge distribution of different isotopes. The MS plays a dominated role in the isotope shifts of light elements and then decreases rapidly with the increase of mass number. By contrast, the FS is dominant for heavy elements.[1] By studying IS, the difference between the mean-square nuclear charge radii and nuclear deformation could be obtained.[2,3] Meanwhile, it has recently been demonstrated that the measurements of nonlinear isotope shift can be used to search for the new boson.[4,5] Experimentally, the IS can be measured by muonic atoms method,[6] electron scattering,[7] x-ray[8] as well as laser spectroscopy.[9] Among these methods, the laser spectroscopy makes it possible to measure stable and radioactive isotopes.[10] From the IS observation and sophisticated theoretical calculation, the nucleus information could be deduced, which provides a new possibility to understand the nuclear effects on atoms. However, due to the high sensitivity of IS parameters to electron correlation, especially for neutral atoms and ions, the determination of the parameters is a great challenge for the atomic theory. The effect of the FS on the isotope shifts of light atoms is small compared with the total IS, separating the tiny FS from the light elements is a complex task that can only be performed on very simple and stable atoms or ions. Therefore, the experiment and theory must have high precision and accuracy in the determination of the radii difference of the light multi-electron isotope.[11] In the past two decades, Artemyev *et al.* calculated the relativistic nuclear recoil corrections of low-lying states for H-like ions by using the B-spline method for the Dirac equation.[12,13] The numerical results were presented for the IS of the lowest-lying states of helium atoms by Pachucki *et al.*,[14] and the relativistic nuclear recoil corrections of He-like ions were calculated by Shabaev and Zubova *et al.*[15,16] As far as Li-like ions are concerned, most of researches have been done on lithium atoms,[1,17] and some isotope shifts of low-lying levels along the lithium isoelectronic sequence were also calculated. For example, Li *et al.* and Zubova *et al.* calculated and discussed the relativistic mass- and field-shift parameters based on the MCDHF and large-scale configuration interaction Dirac–Fock–Sturm (CI-DFS) methods, respectively.[18,19] Kozhedub *et al.* recently calculated the relativistic mass shift for the $2p_{1/2} \rightarrow 2s$ and $2p_{3/2} \rightarrow 2s$ transitions along the Li-like isoelectronic sequence.[20] Zubova *et al.* calculated the isotope shifts in Be-like thorium and uranium ions by using the CI-DFS method. Xiang Zhang *et al.* calculated the field shift and mass shift parameters in Be-like ions by using the MCDHF and RCI methods.[21,22] The isotope shifts of the $2p_{3/2} \rightarrow 2p_{1/2}$ transition in B-like ions were evaluated by using a large-scale CI-DFS method by Zubova *et al.*[23] Recently, Silwal *et al.* have extended their study to the complex electronic systems such as Na-like, Mg-like, and Al-like ions.[24,25]

Calcium is an essential element for metabolism and the

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fifth most abundant elements in the Earth's crust. Calcium and its ions produce strong spectral lines in the atmospheres of the sun and other stars. Their shape are strongly influenced by IS.[26] For decades, hyperfine structure and IS in various transitions of calcium isotopes have been studied theoretically[27,28] and experimentally.[29,30] This element is also widely used in biomedicine, planetary science, archeology, and other fields.[31] Ca has six stable isotopes which are ^{40}Ca, ^{42}Ca, ^{43}Ca, ^{44}Ca, ^{46}Ca, and ^{48}Ca, the abundances are 96.9%, 0.647%, 0.135%, 2.09%, 0.004%, and 0.187%, respectively.

In this work, the contributions of the MS, FS, and IS of Li-like Ca ions are calculated by using MCDHF methods. The electronic correlation effects on the MS, FS, and IS are included by systematically increasing the active space to $n \leq 8$ to take the electron correlation effects into account efficiently. A separated relativistic configuration interaction calculation is performed to include the Breit-interaction and quantum electrodynamics (QED) contributions(such as, self-energy corrections and vacuum polarization) which are important for the highly charged ions. Finally, the IS on the transition wavelength are calculated.

2. Theory and computational methodology

The relativistic MCDHF method is one of the most widely used methods for study on the complex atomic structure and properties research.[32–38] The GRASP family codes are based on the MCDHF method which developed in the past 40 years.[39–44] The present work is performed by newly developed GRASP2K[43] and RIS4 package.[45] The detailed theory was expounded in the monograph of I. P. Grant.[46] Only a brief description on the method is given below.

In the MCDHF method, the atomic state wave function (ASFs) $\Psi(\gamma PJM_J)$ can be expressed in terms of configuration state functions (CSFs) $\Phi(\gamma_\nu PJM_J)$ with same parity P, total angular momentum J, and its z component M_J, i.e.,

$$\Psi(\gamma PJM_J) = \sum_{\nu=1}^{N} c_\nu \Phi(\gamma_\nu PJM_J), \tag{1}$$

where N is the number of CSFs, c_ν is the expansion coefficient for the state ν, γ and γ_ν represent all additional quantum numbers in addition to the parity P, total angular momentum J, and its z component M_J to defines the state uniquely. The CSFs are built from the antisymmetric products of one-electron Dirac orbital. These one-electron Dirac orbital and the expansion coefficients c_ν in CSFs are obtained by using the relativistic self-consistent field procedure. The MCDHF calculations are followed by the RCI, the Breit interaction and QED correction are included as perturbations in a separated RCI calculations by using GRASP2K package.

The isotope shift of the level i, $E_{i,\mathrm{IS}}^{A,A'}$, between two isotopes A and A' can be given by

$$\delta E_{i,\mathrm{IS}}^{A,A'} = \delta E_{i,\mathrm{MS}}^{A,A'} + \delta E_{i,\mathrm{FS}}^{A,A'}, \tag{2}$$

where $\delta E_{i,\mathrm{MS}}^{A,A'}$ and $\delta E_{i,\mathrm{FS}}^{A,A'}$ represent the mass shift (MS) and field shift (FS) between A and A', respectively. The mass shift can usually be written as the sum of normal mass shift (NMS) $\delta E_{i,\mathrm{NMS}}^{A,A'}$ and specific mass shift (SMS) $\delta E_{i,\mathrm{SMS}}^{A,A'}$

$$\delta E_{i,\mathrm{MS}}^{A,A'} = \delta E_{i,\mathrm{NMS}}^{A,A'} + \delta E_{i,\mathrm{SMS}}^{A,A'}, \tag{3}$$

NMS and SMS corresponding to the one-body and two-body nuclear-recoil terms in the relativistic Hamiltonian, respectively. The MS contribution can be further written as

$$\begin{aligned}\delta E_{i,\mathrm{MS}}^{A,A'} &= \left(\frac{M'-M}{MM'}\right)(K_{i,\mathrm{NMS}} + K_{i,\mathrm{SMS}}) \\ &= \left(\frac{M'-M}{MM'}\right) K_{i,\mathrm{MS}},\end{aligned} \tag{4}$$

where M and M' are the nuclear masses of the isotopes A and A', respectively. $K_{i,\mathrm{NMS}}$ and $K_{i,\mathrm{SMS}}$ represent the NMS parameters and SMS parameters obtained in the $(\alpha Z)^4 m^2/M$ approximation from the following expectation values:

$$\frac{K_{i,\mathrm{NMS}}}{M} = \langle \Psi_i(\gamma PJM_J)|\hat{H}_{\mathrm{NMS}}|\Psi_i(\gamma PJM_J)\rangle, \tag{5}$$

$$\frac{K_{i,\mathrm{NMS}}}{M} = \langle \Psi_i(\gamma PJM_J)|\hat{H}_{\mathrm{SMS}}|\Psi_i(\gamma PJM_J)\rangle. \tag{6}$$

The Hamiltonians $\hat{H}_{\mathrm{NMS}}$ and $\hat{H}_{\mathrm{SMS}}$ are given by

$$\hat{H}_{\mathrm{NMS}} = \frac{1}{2M}\sum_{i=1}^{N}\left[\boldsymbol{p}_i^2 - \frac{\alpha Z}{r_i}\boldsymbol{\alpha}_i\cdot\boldsymbol{p}_i - \frac{\alpha Z}{r_i}\frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\cdot\boldsymbol{p}_i\right], \tag{7}$$

$$\hat{H}_{\mathrm{SMS}} = \frac{1}{2M}\sum_{i\neq j}^{N}\left[\boldsymbol{p}_i\cdot\boldsymbol{p}_j - \frac{\alpha Z}{r_i}\boldsymbol{\alpha}_i\cdot\boldsymbol{p}_j - \frac{\alpha Z}{r_i}\frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\cdot\boldsymbol{p}_j\right], \tag{8}$$

where $\boldsymbol{p}_i$ and $\boldsymbol{p}_j$ are the momentum operator of the i-th electron and j-th electron, respectively. $\boldsymbol{r}$ is the position vector, $r = |\boldsymbol{r}|$, $\boldsymbol{\alpha}_i$ are the Dirac matrices and α is the fine structure constant, Z and M are the nuclear charge number and nuclear mass, respectively. From the expression of the Hamiltonian above, the mass shift parameters can be decomposed into three parts

$$K_{i,\mathrm{NMS}} = K_{i,\mathrm{NMS}}^{(1)} + K_{i,\mathrm{NMS}}^{(2)} + K_{i,\mathrm{NMS}}^{(3)}, \tag{9}$$

$$K_{i,\mathrm{SMS}} = K_{i,\mathrm{SMS}}^{(1)} + K_{i,\mathrm{SMS}}^{(2)} + K_{i,\mathrm{SMS}}^{(3)}, \tag{10}$$

where the $K^{(1)}$ term is generally referred to as the non-relativistic contribution and the sum of the last two terms, written as $K^{(2)+(3)}$, are the lowest-order relativistic correction in the Breit approximation. Considering a transition k connecting the upper level u and lower level l, the line frequency isotope mass shift can be expressed as

$$\delta\nu_{k,\mathrm{MS}}^{A,A'} = \left(\frac{M'-M}{MM'}\right)\frac{\Delta K_{\mathrm{MS}}}{h}, \tag{11}$$

where $\Delta K_{\mathrm{MS}} = (K_{\mathrm{u,MS}} - K_{\mathrm{l,MS}})$ is the line mass shift param-

eters between the upper (u) and lower (l) levels. Field shift parameter F_i for the state i can be given by[47]

$$F_i = \frac{Z}{3\hbar}\left(\frac{e^2}{4\pi\varepsilon_0}\right)|\Psi(0)|^2, \tag{12}$$

where the $|\Psi(0)|^2$ is the total electron probability density at the origin. So the line frequency field shift for the transition k can be approximated as

$$\delta\nu_{k,\mathrm{FS}}^{A,A'} \approx \Delta F_k \delta\langle r^2\rangle^{A,A'}, \tag{13}$$

where $\Delta F_k = (F_\mathrm{u} - F_\mathrm{l})$ is the line field shift parameter between the upper (u) and lower (l) levels, and $\delta\langle r^2\rangle^{A,A'}$ is the difference between the mean-square nuclear charge radius of A and A'. Therefore, the IS on the wavelength of the transition k from different isotopes can be estimated.

3. Electron correlation model and calculation strategy

The isotope shift is sensitive to the electron correlation effects. In order to take the electron correlation effects into account efficiently, an electron correlation model is constructed by using active space method in this work. The reference configurations of Li-like Ca ions are $1s^22s$ and $1s^22p$ for the ground and the first excited states, respectively. The Dirac–Fock (DF) wave functions are firstly calculated for the ^{40}Ca isotope. The active space method is used to generate configuration space systematically. The active space is extended up to $n \leq 8$ with single and double excitation from the reference configuration in the present calculation. The electron correlation model is labeled as $nn'll'$. For example, $n4l3$ represents that the correlation configuration space consists of all the single and double excitation from {1s,2s,2p} orbital within $n = 1$ to 4 and $l = 0$ to 3, respectively (n represents the principal quantum number and l stands for the orbital angular momentum quantum number ($l_{\max} = 6$)). The active space is enlarged layer by layer until the physical quantities under investigation converged. For each iteration, only the newly added layer is optimized.

4. Results and discussion

The total energy and excitation energy of 2s ^{2}S$_{1/2}$ and 2p ^{2}P$_{1/2,3/2}$ transitions of Li-like Ca ions from the different electron correlation models are given in Table 1. It can be found that the total energy and the excitation energy relative to the ground state tends to be converged with the increase of the active space, respectively. Comparing our results with the data from NIST database,[48] the relative difference between two results are about 0.04% and 0.03% for the 2p ^{2}P$_{1/2}$ and 2p ^{2}P$_{3/2}$, respectively. This indicates that the most important electron correlation effects are included in the present calculation.

Table 1. Total energy of 2s ^{2}S$_{1/2}$, 2p ^{2}P$_{1/2,3/2}$ and the excitation energy relative to 2s ^{2}S$_{1/2}$ in Li-like Ca ions.

	Total energy (Hartree)			Excitation energy (eV)	
	2s ^{2}S$_{1/2}$	2p ^{2}P$_{1/2}$	2p ^{2}P$_{3/2}$	2p ^{2}P$_{1/2}$	2p ^{2}P$_{3/2}$
DF	−431.9885	−430.6616	−430.4760	36.1064	41.1594
$n2l1$	−432.0150	−430.6775	−430.4918	36.3955	41.4482
$n3l2$	−432.0376	−430.7120	−430.5258	36.0727	41.1390
$n4l3$	−432.0431	−430.7200	−430.5338	36.0035	41.0697
$n5l4$	−432.0452	−430.7228	−430.5366	35.9848	41.0511
$n6l5$	−432.0462	−430.7240	−430.5378	35.9790	41.0453
$n7l6$	−432.0467	−430.7246	−430.5384	35.9759	41.0421
$n8l6$	−432.0470	−430.7249	−430.5388	35.9755	41.0417
NIST (eV)				35.9625	41.0286

The calculated wavelengths and transition probabilities for the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2,3/2}$ transitions are given in Table 2 with other available data. In this table, λ is the transition wavelength (in Å), A_B and A_C are the transition probability in the Babushkin and Coulomb gauges, which is corresponding to the length and velocity gauge in non-relativistic quantum mechanics, respectively. It can be found that the wavelengths calculated in present work are in good agreement with the values of previous work.[49–51] The consistency of the transition probability from two different gauge is fairly good, which indicate that the wave function used in the present work is good in some extent. It can also be found that the transition probabilities in this work are in good agreement with many-body perturbation theory (MBPT) by Johnson *et al.* and relativistic coupled-cluster method (RCC) by Das *et al.* Although the methods used are different, the electronic correlation effect, Breit interaction and QED correction are almost same. This lead to a good agreement. The agreement of the transition wavelength and probability also indicates the validation of the electron correlation model used in this work.

Table 2. Calculated wavelengths (in Å) and transition probabilities (s^{-1}) for the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$ and 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$ transitions in Li-like Ca ions. Numbers in square brackets designate powers of 10.

	2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$			2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$		
	λ (Å)	A_C (s^{-1})	A_B (s^{-1})	λ (Å)	A_C (s^{-1})	A_B (s^{-1})
Present work	344.64	1.315[9]	1.305[9]	302.09	1.961[9]	1.954[9]
Doschek1 *et al.*[49]	344.77			302.21		
Johnson *et al.*[50]	344.76		1.302[9]	302.19		1.952[9]
Das *et al.*[51]	344.39		1.3(2)[9][a]	300.20		2.00(3)[9][a]

[a]The uncertainties are given in parentheses by Das *et al.*

The NMS, SMS parameters (in GHz u) and FS parameters (in GHz/fm^2) of the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2,3/2}$ transitions of Li-like Ca ions from different correlation models are given in Table 3. The result shows a good convergency with the increase of active space. For the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$ transition, the MS and FS parameters of *n*6*l*5 differ by 0.0087% and 0.0349% from that of *n*7*l*6, while at *n*7*l*6 only differ by 0.0090% and 0.0159% from that of *n*8*l*6. For the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$ transition MS and FS parameters of *n*6*l*5 differ by 0.0107% and 0.0380% from that of *n*7*l*6, while at *n*7*l*6 only differ by 0.0215% and 0.0159% from that of *n*8*l*6. The electron correlation contribution for these parameters increases significantly from DF calculation to *n*3*l*2, and then converges gradually. This means the electron correlation effects have significant contribution to the MS and FS parameters. Additionally, we also compare our results with other available theoretical calculations.[20] There are about 0.8% difference between the present work and the results calculated by Kozhedub *et al.*[20] This difference are mainly come from the different treatment on the electron correlation.

Table 3. NMS, SMS parameters and FS parameters of the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2,3/2}$ transitions of Li-like Ca ions under different correlation models.

	$\Delta K_{\rm NMS}$ (GHz, u)	$\Delta K_{\rm SMS}$ (GHz, u)	$\Delta K_{\rm MS}$ (GHz, u)	ΔF (GHz/fm^2)
	2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$			
DF	−4755.805	−91801.754	−96557.559	−31.476
*n*2*l*1	−5685.847	−101547.550	−107233.390	−31.935
*n*3*l*2	−4884.473	−91528.635	−96413.108	−31.445
*n*4*l*3	−4912.365	−91379.383	−96291.748	−31.509
*n*5*l*4	−4892.667	−91337.198	−96229.865	−31.471
*n*6*l*5	−4894.621	−91312.526	−96207.147	−31.487
*n*7*l*6	−4893.463	−91305.302	−96198.765	−31.476
*n*8*l*6	−4894.898	−91295.180	−96190.078	−31.481
Kozhedub *et al.*[20]			−96980(4)	
	2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$			
DF	−5437.290	−92071.883	−97509.173	−31.583
*n*2*l*1	−6272.999	−101811.360	−108084.360	−31.992
*n*3*l*2	−5417.450	−91998.924	−97416.374	−31.513
*n*4*l*3	−5427.687	−91810.913	−97238.600	−31.572
*n*5*l*4	−5395.612	−91773.261	−97168.873	−31.535
*n*6*l*5	−5392.242	−91742.346	−97134.588	−31.552
*n*7*l*6	−5386.289	−91737.887	−97124.176	−31.540
*n*8*l*6	−5384.545	−91718.771	−97103.316	−31.545
Kozhedub *et al.*[20]			−97870(4)	

The shifts of the wavelength relative to the wavelength of ^{A,40}Ca due to MS, FS and IS (in units of fm) of the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$ and 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$ transitions in Li-like Ca ions for the isotopes (A = 40, 42, 43, 44, 46, 48) are given in Table 4. It can be found that the contribution of the MS is obviously larger than that of FS. The MS contribution, which mainly comes from the SMS, grows rapidly with the increase of mass number, while the FS contribution remains almost unchanged. It can be concluded that the IS on calcium almost completely comes from MS, while the contribution of FS to IS is negligible small. Li *et al.*[18] found the MS is dominant in IS for $6 \le Z \le 34$ elements, which agrees with the present calculations. They also suggest that the situation to might be inversed for heavy elements with $Z \ge 35$. For these isotopes, the largest contribution is IS of Ca^{48,40} and the most prominent shifts is about 0.01Å which is possible to be observed in the experimental observation. For the convenience to the experimentalists, the IS on the transition wavelength in the units of meV are given in Fig. 1.

Table 4. Calculated wavelength values of the MS, FS and IS (in units of fm) of the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$ and 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$ transitions in Li-like Ca ions for the isotope pair ^{A,40}Ca. The FS is calculated by using the evaluated value $\delta\langle r^2\rangle$ in Ref. [52].

Mass number	NMS	SMS	MS	FS	IS
		2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$			
42	−23.0867	−430.5918	−453.6784	26.5773	−427.1011
43	−33.8247	−630.8670	−664.6917	15.4777	−649.2140
44	−44.0746	−822.0388	−866.1134	35.1574	−830.9560
46	−63.2374	−1179.4470	−1242.6844	15.3904	−1227.2940
48	−80.8034	−1507.0711	−1587.8745	−0.4365	−1588.3111
		2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$			
42	−19.5133	−332.3846	−351.8980	20.4628	−331.4351
43	−28.5893	−486.9821	−515.5714	11.9168	−503.6546
44	−37.2527	−634.5524	−671.8052	27.0689	−644.7362
46	−53.4496	−910.4448	−963.8944	11.8496	−952.0448
48	−68.2967	−1163.3461	−1231.6428	−0.3361	−1231.9789

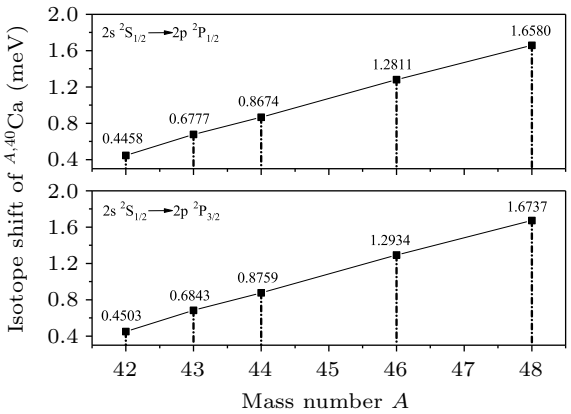


Fig. 1. The values of the IS for the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$ and 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$ transitions in Li-like Ca ions for the isotope pair ^{A,40}Ca.

5. Conclusion

In conclusion, the parameters of MS and FS as well as IS for the 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2,3/2}$ transitions of Li-like Ca ions are calculated by using the MCDHF method. The wavelengths of the MS, FS and IS (in units of fm) of the Li-like 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{1/2}$ and 2s ^{2}S$_{1/2}$ → 2p ^{2}P$_{3/2}$ transitions for the isotope pair ^{A,40}Ca (A = 40, 42, 43, 44, 46, 48) are calculated. The field shift is calculated using the evaluated value of $\delta\langle r^2\rangle$ by Ref. [52]. It is found that the Li-like Ca ions have a most prominent shift about 0.01 Å, which is easier to observe experimentally.

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