PHYSICAL REVIEW A **87**, 023402 (2013)

Magic wavelengths for trapping the alkali-metal atoms with circularly polarized light

B. K. Sahoo
Theoretical Physics Division, Physical Research Laboratory, Navrangpura, Ahmedabad-380009, India

Bindiya Arora[*]
Department of Physics, Guru Nanak Dev University, Amritsar, Punjab-143005, India

(Received 7 November 2012; revised manuscript received 3 December 2012; published 5 February 2013)

Magic wavelengths for the Li, Na, and K alkali-metal atoms are determined using the circularly polarized light for the ns-$np_{1/2,3/2}$ transitions, with n denoting their ground-state principal quantum numbers, by studying their differential ac dynamic polarizabilities. These wavelengths for all possible sublevels are given linearly as well as circularly polarized lights and are further compared with the available results for the linearly polarized light. The present study suggests that it is possible to carry out state-insensitive trapping of different alkali-metal atoms using the circularly polarized light.

DOI: 10.1103/PhysRevA.87.023402 PACS number(s): 37.10.Gh, 32.10.Dk, 06.30.Ft, 32.80.−t

I. INTRODUCTION

It has been known for some time that atoms can be trapped and manipulated by the gradient forces of light waves [1–3]. However, for any two internal states of an atom, the Stark shifts caused due to the trap light are different, which affects the fidelity of the experiments [4,5]. Katori *et al.* [6] suggested a solution to this problem that the trapping laser can be tuned to a wavelength, λ_{magic}, where the differential ac Stark shifts of the transition vanish. Knowledge of magic wavelengths is necessary in many areas of physics. In particular, these wavelengths have unavoidable application for atomic clocks and quantum computing [7,8]. For example, a major concern for the accuracy of optical lattice clocks is the ability to cancel the large light shifts created by the trapping potential of the lattice. Similarly, for most quantum computational schemes, it is often desirable to optically trap the neutral atoms without affecting the internal energy-level spacing for the atoms.

Over the years, there has been quite a large number of calculations of the magic wavelengths of alkali-metal atoms for linearly polarized traps [9–11], with rather fewer calculations of the magic wavelength for the circularly polarized traps. Moreover, as stated in [11], the linearly polarized lattice scheme offers only a few cases in which the magic wavelengths are of experimental relevance. Therefore, we would like to explore the idea of using the circularly polarized light. Using the circularly polarized light may be advantageous owing to the dominant role played by vector polarizabilities in estimating the ac Stark shifts [12–14]. These polarizability contributions are absent in the linearly polarized light. Recently, we investigated the magic wavelengths for the circularly polarized light in rubidium (Rb) atoms and found spectacular results that can lead to state-insensitive trapping of Rb atoms using this light [12]. In this paper, we aim to search for magic wavelengths in the Li, Na, and K atoms due to circularly polarized light and also compare our results for linearly polarized light with other available results.

II. THEORY

The energy shift of any state v of an atom placed in a frequency-dependent ac electric field $\mathcal{E}(\omega)$ can be estimated from the time-independent perturbation theory at the second-order perturbation level as

$$\Delta E_v \simeq -\tfrac{1}{2}\alpha_v(\omega)\mathcal{E}^2, \tag{1}$$

where $\alpha_v(\omega)$ is the dynamic dipole polarizability of the atom in the vth state and can be expressed as

$$\alpha_v(\omega) = -\sum_{k\neq v}(p^*)_{vk}(p)_{kv}\left[\frac{1}{\delta E_{vk}+\omega}+\frac{1}{\delta E_{vk}-\omega}\right], \tag{2}$$

where $(p)_{kv} = \langle\psi_k|D|\psi_v\rangle$ is the electric-dipole matrix element. In a more conventional form, the dipole polarizability $\alpha(\omega)$ can be decomposed into three components as

$$\alpha_v(\omega) = \alpha_v^0(\omega) + \mathcal{A}\cos\theta_k\frac{m_j}{j}\alpha_v^1(\omega) + \left\{\frac{3\cos^2\theta_p-1}{2}\right\}\frac{3m_j^2-j(j+1)}{j(2j-1)}\alpha_v^2(\omega), \tag{3}$$

which separates out the m_j-dependent and -independent components. The m_j-independent parameters $\alpha_0(\omega)$, $\alpha_1(\omega)$, and $\alpha_2(\omega)$ are known as scalar, vector, and tensor polarizabilities, respectively. They are given in terms of the reduced matrix dipole matrix elements as [15]

$$\alpha_v^0(\omega) = \frac{1}{3(2j_v+1)}\sum_{j_k}|\langle\psi_v\parallel D\parallel\psi_k\rangle|^2 \times\left[\frac{1}{\delta E_{kv}+\omega}+\frac{1}{\delta E_{kv}-\omega}\right], \tag{4}$$

$$\alpha_v^1(\omega) = -\sqrt{\frac{6j_v}{(j_v+1)(2j_v+1)}}\sum_{j_k}\begin{Bmatrix} j_v & 1 & j_v\\ 1 & j_k & 1\end{Bmatrix} \times(-1)^{j_v+j_k+1}|\langle\psi_v\parallel D\parallel\psi_k\rangle|^2 \times\left[\frac{1}{\delta E_{kv}+\omega}-\frac{1}{\delta E_{kv}-\omega}\right], \tag{5}$$

---

[*] arorabindiya@gmail.com

TABLE I. Absolute values of $E1$ matrix elements in Li, Na, and K atoms in ea_0 using CCSD(T) methods. Uncertainties in the CCSD(T) results are given in the parentheses.

Transition	CCSD(T)	Transition	CCSD(T)
		Li	
$2s_{1/2} \rightarrow 2p_{1/2}$	3.318(4)	$2p_{1/2} \rightarrow 5d_{3/2}$	1.212(1)
$2s_{1/2} \rightarrow 3p_{1/2}$	0.182(2)	$2p_{1/2} \rightarrow 6d_{3/2}$	0.767(1)
$2s_{1/2} \rightarrow 4p_{1/2}$	0.159(2)	$2p_{1/2} \rightarrow 7d_{3/2}$	0.566(5)
$2s_{1/2} \rightarrow 5p_{1/2}$	0.119(4)	$2p_{3/2} \rightarrow 3s_{1/2}$	3.445(3)
$2s_{1/2} \rightarrow 6p_{1/2}$	0.092(2)	$2p_{3/2} \rightarrow 4s_{1/2}$	0.917(2)
$2s_{1/2} \rightarrow 7p_{1/2}$	0.072(1)	$2p_{3/2} \rightarrow 5s_{1/2}$	0.493(2)
$2s_{1/2} \rightarrow 2p_{3/2}$	4.692(5)	$2p_{3/2} \rightarrow 6s_{1/2}$	0.326(2)
$2s_{1/2} \rightarrow 3p_{3/2}$	0.257(2)	$2p_{3/2} \rightarrow 7s_{1/2}$	0.233(2)
$2s_{1/2} \rightarrow 4p_{3/2}$	0.225(2)	$2p_{3/2} \rightarrow 3d_{3/2}$	2.268(2)
$2s_{1/2} \rightarrow 5p_{3/2}$	0.169(4)	$2p_{3/2} \rightarrow 4d_{3/2}$	0.863(1)
$2s_{1/2} \rightarrow 6p_{3/2}$	0.130(2)	$2p_{3/2} \rightarrow 5d_{3/2}$	0.502(1)
$2s_{1/2} \rightarrow 7p_{3/2}$	0.102(1)	$2p_{3/2} \rightarrow 6d_{3/2}$	0.344(1)
$2p_{1/2} \rightarrow 3s_{1/2}$	2.436(3)	$2p_{3/2} \rightarrow 7d_{3/2}$	0.253(4)
$2p_{1/2} \rightarrow 4s_{1/2}$	0.648(3)	$2p_{3/2} \rightarrow 3d_{5/2}$	6.805(1)
$2p_{1/2} \rightarrow 5s_{1/2}$	0.349(3)	$2p_{3/2} \rightarrow 4d_{5/2}$	2.589(1)
$2p_{1/2} \rightarrow 6s_{1/2}$	0.231(2)	$2p_{3/2} \rightarrow 5d_{5/2}$	1.505(1)
$2p_{1/2} \rightarrow 7s_{1/2}$	0.165(2)	$2p_{3/2} \rightarrow 6d_{5/2}$	1.031(1)
$2p_{1/2} \rightarrow 3d_{3/2}$	5.072(1)	$2p_{3/2} \rightarrow 7d_{5/2}$	0.746(5)
$2p_{1/2} \rightarrow 4d_{3/2}$	1.929(1)		
		Na	
$3s_{1/2} \rightarrow 3p_{1/2}$	3.545(3)	$3p_{1/2} \rightarrow 5d_{3/2}$	0.997(2)
$3s_{1/2} \rightarrow 4p_{1/2}$	0.304(2)	$3p_{1/2} \rightarrow 6d_{3/2}$	0.645(1)
$3s_{1/2} \rightarrow 5p_{1/2}$	0.107(1)	$3p_{1/2} \rightarrow 7d_{3/2}$	0.460(1)
$3s_{1/2} \rightarrow 6p_{1/2}$	0.056(2)	$3p_{3/2} \rightarrow 4s_{1/2}$	5.070(4)
$3s_{1/2} \rightarrow 7p_{1/2}$	0.035(2)	$3p_{3/2} \rightarrow 5s_{1/2}$	1.072(2)
$3s_{1/2} \rightarrow 8p_{1/2}$	0.026(2)	$3p_{3/2} \rightarrow 6s_{1/2}$	0.553(2)
$3s_{1/2} \rightarrow 3p_{3/2}$	5.012(4)	$3p_{3/2} \rightarrow 7s_{1/2}$	0.360(1)
$3s_{1/2} \rightarrow 4p_{3/2}$	0.434(2)	$3p_{3/2} \rightarrow 8s_{1/2}$	0.255(1)
$3s_{1/2} \rightarrow 5p_{3/2}$	0.153(2)	$3p_{3/2} \rightarrow 3d_{3/2}$	3.048(3)
$3s_{1/2} \rightarrow 6p_{3/2}$	0.081(2)	$3p_{3/2} \rightarrow 4d_{3/2}$	0.856(2)
$3s_{1/2} \rightarrow 7p_{3/2}$	0.051(2)	$3p_{3/2} \rightarrow 5d_{3/2}$	0.445(2)
$3s_{1/2} \rightarrow 8p_{3/2}$	0.037(2)	$3p_{3/2} \rightarrow 6d_{3/2}$	0.288(1)
$3p_{1/2} \rightarrow 4s_{1/2}$	3.578(4)	$3p_{3/2} \rightarrow 7d_{3/2}$	0.205(1)
$3p_{1/2} \rightarrow 5s_{1/2}$	0.758(3)	$3p_{3/2} \rightarrow 3d_{5/2}$	9.144(4)
$3p_{1/2} \rightarrow 6s_{1/2}$	0.391(2)	$3p_{3/2} \rightarrow 4d_{5/2}$	2.570(3)
$3p_{1/2} \rightarrow 7s_{1/2}$	0.255(2)	$3p_{3/2} \rightarrow 5d_{5/2}$	1.336(2)
$3p_{1/2} \rightarrow 8s_{1/2}$	0.180(1)	$3p_{3/2} \rightarrow 6d_{5/2}$	0.864(2)
$3p_{1/2} \rightarrow 3d_{3/2}$	6.807(3)	$3p_{3/2} \rightarrow 7d_{5/2}$	0.606(2)
$3p_{1/2} \rightarrow 4d_{3/2}$	1.916(2)		
		K	
$4s_{1/2} \rightarrow 4p_{1/2}$	4.131(20)	$4p_{1/2} \rightarrow 6d_{3/2}$	0.293(5)
$4s_{1/2} \rightarrow 5p_{1/2}$	0.282(6)	$4p_{1/2} \rightarrow 7d_{3/2}$	0.261(4)
$4_{1/2} \rightarrow 6p_{1/2}$	0.087(5)	$4p_{1/2} \rightarrow 8d_{3/2}$	0.221(4)
$4s_{1/2} \rightarrow 7p_{1/2}$	0.041(5)	$4p_{3/2} \rightarrow 5s_{1/2}$	5.524(10)
$4s_{1/2} \rightarrow 8p_{1/2}$	0.023(3)	$4p_{3/2} \rightarrow 6s_{1/2}$	1.287(10)
$4s_{1/2} \rightarrow 9p_{1/2}$	0.016(3)	$4p_{3/2} \rightarrow 7s_{1/2}$	0.677(6)
$4s_{1/2} \rightarrow 4p_{3/2}$	5.841(20)	$4p_{3/2} \rightarrow 9s_{1/2}$	0.317(5)
$4s_{1/2} \rightarrow 5p_{3/2}$	0.416(6)	$4p_{3/2} \rightarrow 10s_{1/2}$	0.242(5)
$4s_{1/2} \rightarrow 6p_{3/2}$	0.132(6)	$4p_{3/2} \rightarrow 3d_{3/2}$	3.583(20)
$4s_{1/2} \rightarrow 7p_{3/2}$	0.064(5)	$4p_{3/2} \rightarrow 4d_{3/2}$	0.088(5)
$4s_{1/2} \rightarrow 8p_{3/2}$	0.038(3)	$4p_{3/2} \rightarrow 5d_{3/2}$	0.124(5)
$4s_{1/2} \rightarrow 9p_{3/2}$	0.027(3)	$4p_{3/2} \rightarrow 6d_{3/2}$	0.135(5)
$4p_{1/2} \rightarrow 5s_{1/2}$	3.876(10)	$4p_{3/2} \rightarrow 7d_{3/2}$	0.119(4)
$4p_{1/2} \rightarrow 6s_{1/2}$	0.909(10)	$4p_{3/2} \rightarrow 8d_{3/2}$	0.101(3)
$4p_{1/2} \rightarrow 7s_{1/2}$	0.479(5)	$4p_{3/2} \rightarrow 3d_{5/2}$	10.749(50)

TABLE I. (*Continued.*)

Transition	CCSD(T)	Transition	CCSD(T)
$4p_{1/2} \rightarrow 8s_{1/2}$	0.316(5)	$4p_{3/2} \rightarrow 4d_{5/2}$	0.260(5)
$4p_{1/2} \rightarrow 9s_{1/2}$	0.225(3)	$4p_{3/2} \rightarrow 5d_{5/2}$	0.374(5)
$4p_{1/2} \rightarrow 10s_{1/2}$	0.171(3)	$4p_{3/2} \rightarrow 6d_{5/2}$	0.404(5)
$4p_{1/2} \rightarrow 3d_{3/2}$	7.988(40)	$4p_{3/2} \rightarrow 7d_{5/2}$	0.356(5)
$4p_{1/2} \rightarrow 4d_{3/2}$	0.220(5)	$4p_{3/2} \rightarrow 8d_{5/2}$	0.286(5)
$4p_{1/2} \rightarrow 5d_{3/2}$	0.264(5)		

and

$$\alpha_v^2(\omega) = -2\sqrt{\frac{5j_v(2j_v-1)}{6(j_v+1)(2j_v+1)(2j_v+3)}} \times \sum_{j_k} \begin{Bmatrix} j_v & 2 & j_v \\ 1 & j_k & 1 \end{Bmatrix} (-1)^{j_v+j_k+1} |\langle \psi_v \parallel D \parallel \psi_k \rangle|^2 \times \left[\frac{1}{\delta E_{kv}+\omega} + \frac{1}{\delta E_{kv}-\omega} \right]. \qquad (6)$$

In Eq. (3) $\mathcal{A}$, θ_k, and θ_p define the degree of circular polarization, the angle between the wave vector of the electric field and the z axis, and the angle between the direction of polarization and the z axis, respectively. Without loss of generality, it is assumed that the considered frequencies ω are several linewidths off from the resonance lines and $\mathcal{A} = 1$ for right-handed circularly polarized light and $\mathcal{A} = -1$ for left-handed circularly polarized light. In the absence of the magnetic field (or in a weak magnetic field), we approximate $\cos(\theta_k) = \cos(\theta_p) = 1$.

The differential ac Stark shift for a transition is defined as the difference between the Stark shifts of individual levels which are further calculated from the frequency-dependent polarizabilities:

$$\delta(\Delta E)_{np_i - ns} = \Delta E_{np_i} - \Delta E_{ns} = \tfrac{1}{2}\mathcal{E}^2(\alpha_{ns} - \alpha_{np_i}), \qquad (7)$$

where we have used the total polarizabilities of the respective states and $i = 1/2, 3/2$. Since the external electric field $\mathcal{E}$ is arbitrary, we can locate the frequencies or wavelengths where $\alpha_{np_i} = \alpha_{ns}$ for an atom for the null differential ac Stark shifts, which gives the value of magic wavelengths. In other words, the crossing between the two polarizabilities at various values of wavelengths will correspond to λ_{magic}. As pointed out earlier, it will be experimentally convenient to trap atoms at these wavelengths.

III. PROCEDURE FOR CALCULATIONS

The scalar, vector, and tensor polarizabilities can be written using sum over intermediate states as

$$\alpha_v^\lambda = \sum_{j_k} C_{v,k}^\lambda \frac{|\langle j_v || D || j_k \rangle|^2}{E_v - E_k}, \qquad (8)$$

where $\lambda = 0$, 1, and 2 indicate scalar, vector, and tensor polarizabilities and $C_{v,k}^\lambda$ are their corresponding angular coefficients. In order to apply this formula, it is necessary to determine intermediate k states explicitly. Therefore, contributions

TABLE II. Polarizabilities of the ground and first two excited states in Li, Na, and K (a.u.) from this work compared with the results reported in (a) [26], (b) [27], (c) [28], (d) [11], (e) [29], (f) [30], and (g) [31], (h) derived from Ref. [32] D1 line Stark shift measurements and recommended values for ground-state polarizability from Ref. [28], and (i) reported in Ref. [33].

	ns	$np_{1/2}$	$np_{3/2}$	
Contribution	α_v^0	α_v^0	α_v^0	α_v^2
Li ($n = 2$)				
$2s$		−54.041(4)	−54.031(5)	54.031(5)
$2p_{1/2}$	54.041(4)			
$2p_{3/2}$	108.06(1)			
$3s$		35.288(2)	35.288(2)	−35.288(2)
$3p_{1/2}$	0.078			
$3p_{3/2}$	0.156			
$3d_{3/2}$		114.901(2)	11.488(1)	9.190
$3d_{5/2}$			103.419(2)	−20.684
$4s$		1.528	1.530	−1.530
$4p_{1/2}$	0.051			
$4p_{3/2}$	0.102			
$4d_{3/2}$		12.534(1)	1.254	−2.258
$4d_{5/2}$			11.289	−2.258
$\alpha_v(v)$	0.154	7.63	6.931	−0.627
$\alpha_v(cv)$	~0	~0	~0	~0
$\alpha_v(tail)$	1.2(6)	10(5)	10(5)	−1.7(8)
Present study	164.1(6)	128	127	1.5
Other studies	164.16(5)$^{\text{a}}$	126.97(5)$^{\text{a}}$	126.98(5)$^{\text{a}}$	1.610(26)$^{\text{a}}$
Experiment	164.2(11)$^{\text{b}}$			
Na ($n = 3$)				
$3s$		−53.60(7)	−53.53(7)	53.53(7)
$3p_{1/2}$	53.60(7)			
$3p_{3/2}$	107.06(15)			
$4s$		106.625(9)	107.255(9)	−107.255(9)
$3d_{3/2}$		277.47(2)	27.856(2)	22.285(1)
$3d_{5/2}$			250.71(2)	−50.141(4)
$4p_{1/2}$	0.223			
$4p_{3/2}$	0.455			
$5s$		2.588	2.591	−2.591
$5p_{1/2}$	0.024			
$5p_{3/2}$	0.049			
$4d_{3/2}$		15.266(1)	1.525	1.220
$4d_{5/2}$			13.747	−2.749
$\alpha_v(v)$	0.030	6.647	6.616	−1.479
$\alpha_v(cv)$	~0	-1.3×10^{-4}	-2.6×10^{-4}	~0
$\alpha_v(tail)$	0.08(4)	5(3)	5(3)	−1.5(7)
Present study	162.4(2)	361	362	−88
Other studies	162.6(3)$^{\text{c}}$	359.9$^{\text{d}}$	361.6$^{\text{d}}$	−88.4$^{\text{d}}$
Experiment	162.7(8)$^{\text{e}}$	359.2(6)$^{\text{e}}$	360.4(7)$^{\text{e}}$	−88.3(4)$^{\text{f}}$
K ($n = 4$)				
$4s$		−94.8(2)	−94.3(3)	94.3(3)
$4p_{1/2}$	94.8(2)			
$4p_{3/2}$	188.7(5)			
$5s$		0.027	139.81(3)	−139.81(3)
$3d_{3/2}$		545.9(4)	55.29(2)	44.23(2)
$3d_{5/2}$			497.7(5)	−99.54(10)
$5p_{1/2}$	0.236			
$5p_{3/2}$	0.512			
$4d_{3/2}$		0.246	0.020	0.016
$4d_{5/2}$			0.172	−0.035
$6s$		4.179(1)	4.205(1)	−4.205(1)
$6p_{1/2}$	0.019			
$6p_{3/2}$	0.044			

TABLE II. (*Continued.*)

	ns	$np_{1/2}$	$np_{3/2}$	
Contribution	α_v^0	α_v^0	α_v^0	α_v^2
$5d_{3/2}$		0.296	0.033	0.026
$5d_{5/2}$			0.299	−0.060
$\alpha_v(v)$	0.020	2.421	2.444	−3.160
$\alpha_v(cv)$	−0.13	∼0	∼0	∼0
$\alpha_v(tail)$	0.06(3)	6.1(6)	6.2(6)	−2.1(4)
Present study	289.8(6)	605.3	616.0	−107.5
Other studies	290.2(8)[c]	602[d]	613[d]	−109[d]
Experiment	290.58(1.42)[g]	606.7(6)[h]	614(10)[i]	107(2)[i]

from the intermediate states involving core orbitals cannot be determined in this procedure. For a practical approach, we divide contributions to α_v as

$$\alpha_v^\lambda = \alpha_v^\lambda(c) + \alpha_v^\lambda(vc) + \alpha_v^\lambda(v) \tag{9}$$

by expressing wave functions of state v as a closed core with the corresponding valence orbital so that $\alpha_v^\lambda(c)$ and $\alpha_v^\lambda(vc)$ account for contributions from the intermediate states involving core orbitals and $\alpha_v^\lambda(v)$ take care of the contributions from the excited states involving the virtual orbitals. As a result, $\alpha_v^\lambda(v)$ contributions will be the dominant ones among them and can be estimated determining the important low-lying intermediate states explicitly. Contributions from $\alpha_v^\lambda(c)$, $\alpha_v^\lambda(vc)$, and higher intermediate states with the virtual orbitals (given as *tail* contributions) are obtained using the third-order many-body perturbation theory [MBPT(3) method] in the Lewis-Galgarno approach [12,16].

To determine contributions to $\alpha_v^\lambda(v)$ from the low-lying intermediate states involving virtual orbitals, we express atomic wave functions of a given state with a closed core and a valence orbital k as

$$|\Phi_k\rangle = a_k^\dagger|\Phi_0\rangle, \tag{10}$$

where $|\Phi_0\rangle$ is the Dirac-Fock (DF) wave function for the closed core and $a_k^\dagger$ corresponds to the attachment of the k valence orbital to the core. The wave function of the exact state is then expressed in the coupled-cluster (CC) theory framework as [17]

$$|\Psi_v\rangle = e^T\{1 + S_v\}|\Phi_v\rangle, \tag{11}$$

where T and S_v operators account for correlation effects from the core and the core with valence orbitals, respectively. Amplitudes of these operators are obtained using the Dirac-Coulomb (DC) Hamiltonian, and the detailed procedures are explained elsewhere (e.g., refer to [18–20]).

We calculate the reduced matrix elements of D between states $|\Psi_f\rangle$ and $|\Psi_i\rangle$, after obtaining from the CC method that to be used in the sum-over-states approach, as the expression

$$\langle\Psi_f||D||\Psi_i\rangle = \frac{\langle\Phi_f||\{1 + S_f^\dagger\}\overline{D}\{1 + S_i\}||\Phi_i\rangle}{\sqrt{\mathcal{N}_f\mathcal{N}_i}}, \tag{12}$$

where $\overline{D} = e^{T^\dagger}De^T$ and $\mathcal{N}_v = \langle\Phi_v|e^{T^\dagger}e^T + S_v^\dagger e^{T^\dagger}e^T S_v|\Phi_v\rangle$. Detailed calculation procedures of these expressions are discussed elsewhere [18–20].

IV. RESULTS AND DISCUSSION

We first use the obtained $E1$ matrix elements and other MBPT(3) results to evaluate the static polarizabilities ($\omega = 0$) of the considered states in Li, Na, and K to benchmark their accuracies against the previously reported experimental and theoretical results. The matrix elements calculated using the method mentioned above are shown in Table I and are presented under the columns for coupled-cluster theory with single, double, and partially triple excitations [CCSD(T)]. Uncertainties in the $E1$ matrix elements and MBPT(3) results are estimated using the procedures given in [12,21]. To reduce the uncertainties in our calculations, we have taken the $E1$ matrix elements compiled in Ref. [22] (they are pointed out in Table I explicitly), instead of from our calculations. Experimental energies from the National Institute of Science and Technology (NIST) database [23–25] are used in the present calculations. The determined polarizabilities are given in Table II and are compared with the other results. The most accurate experimental measurement of Li ground-state polarizability $\alpha_{2s}^0 = 164.2(11)$ a.u. was obtained in [27]. Our result $\alpha_{2s}^0 = 164(1)$ a.u. is in excellent agreement with the experimental value. The most stringent experimental value for

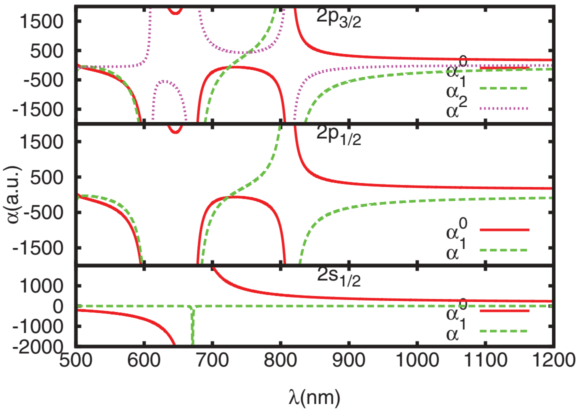

FIG. 1. (Color online) Scalar α^0, vector α^1, and tensor α^2 polarizability (in a.u.) for the $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ states of a Li atom as a function of wavelength (in nm).

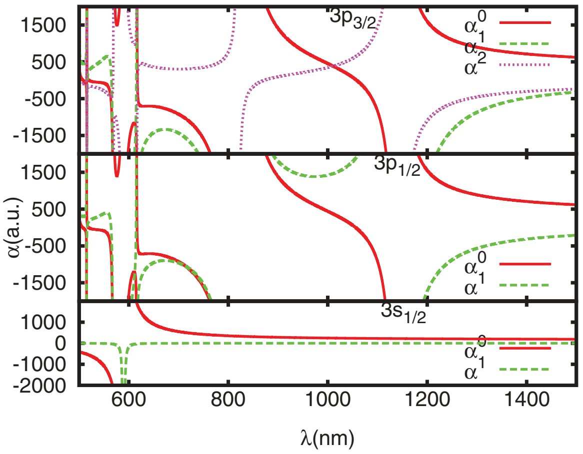

FIG. 2. (Color online) Scalar α^0, vector α^1, and tensor α^2 polarizability (in a.u.) for the $3s_{1/2}$, $3p_{1/2}$, and $3p_{3/2}$ states of a Na atom as a function of wavelength (in nm).

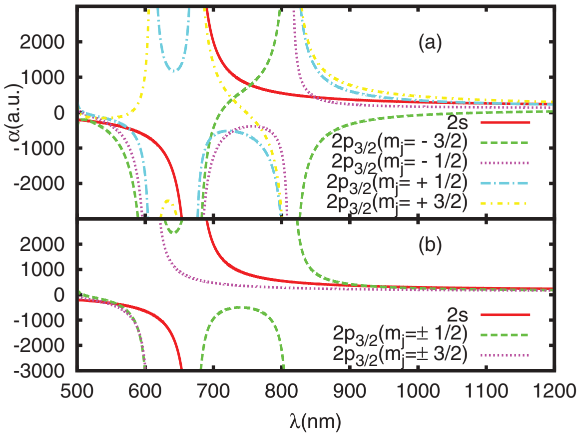

FIG. 4. (Color online) Total dynamic polarizability for $2s$ and $2p_{3/2}$ states of a Li atom due to (a) linearly polarized light and (b) circularly polarized light. The magic wavelength for the corresponding $2s$-$2p_{3/2}$ transition is given by the crossing of two polarizability curves.

Na ground-state polarizability was obtained by interferometry experiments as $\alpha^0_{3s} = 162.7(8)$ a.u. [29], and our present value $\alpha^0_{3s} = 162.4(2)$ a.u. agrees well with the experimental value within the uncertainty limits. The most recent experimental result available for the ground-state polarizability in K is $\alpha^0_{4s} = 290.58(1.42)$ a.u. [31], which is very close to our calculated value $\alpha^0_{4s} = 289.8(6)$ a.u. Our results for all the states in the three considered atoms also agree with other theoretical results. Therefore, the present polarizability results can be used further to find out magic wavelengths in these atoms.

To find magic wavelengths, i.e., the null differential dynamic polarizabilities among various states, we first determine the frequency-dependent polarizabilities. In Figs. 1, 2, and 3, we present these results for the scalar, vector, and tensor polarizabilities for Li, Na, and K atoms, respectively. In Figs. 4, 5, and 6 we plot the total dynamic polarizability for the ns and $np_{3/2}$ states of Li, Na, and K atoms, respectively (where $n = 2$ for Li, $n = 3$ for Na, and $n = 4$ for K). In the case of the $np_{3/2}$ states, the total polarizability in the presence of linearly polarized light is determined as $\alpha = \alpha_0 - \alpha_2$ for $m_j = \pm 1/2$ and $\alpha = \alpha_0 + \alpha_2$ for $m_j = \pm 3/2$. Similarly, the total polarizability for the $np_{3/2}$ states due to the circularly polarized light is determined separately for the $m_j = -3/2, -1/2, 1/2, 3/2$ sublevels using Eq. (3). Magic wavelengths for the corresponding transitions are located at the crossing of the two curves.

In Table III, we list magic wavelengths for the considered atoms in the presence of linearly polarized light. As shown in Table III, the magic wavelengths found in the present work agree very well with previous publications [11,26]. We do not discuss these results in detail here since they are discussed in the above works, and we focus mainly on the results obtained due to the circularly polarized light. It is to be noted that we did not find any other data to compare with our magic wavelength results in the case of K atoms for wavelengths less than 600 nm. We consider hereafter the left-handed circularly polarized light for all the practical purposes as the results will have a similar

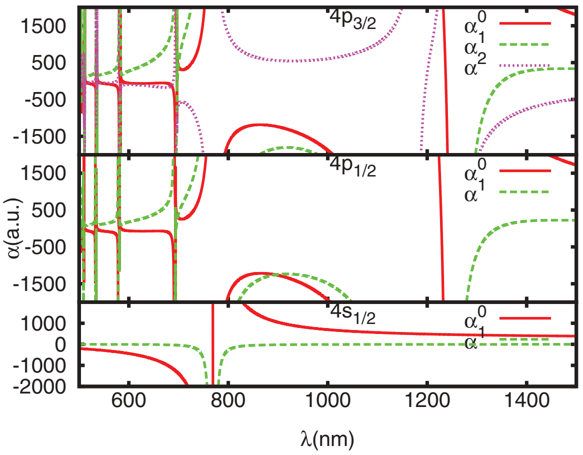

FIG. 3. (Color online) Scalar α^0, vector α^1, and tensor α^2 polarizability (in a.u.) for the $4s_{1/2}$, $4p_{1/2}$, and $4p_{3/2}$ states of a K atom as a function of wavelength (in nm).

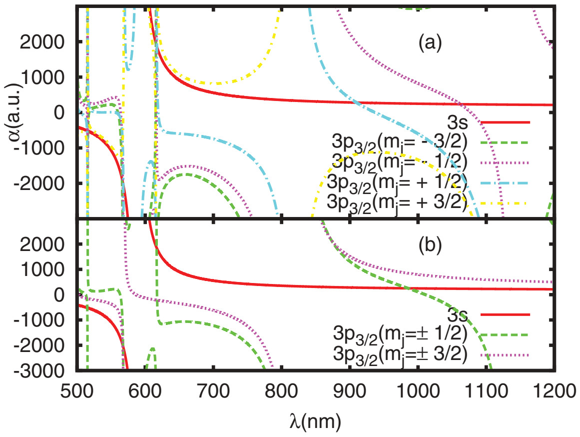

FIG. 5. (Color online) Total dynamic polarizability for $3s$ and $3p_{3/2}$ states of a Na atom due to (a) linearly polarized light and (b) circularly polarized light. The magic wavelength for the corresponding $3s$-$3p_{3/2}$ transition is given by the crossing of two polarizability curves.

TABLE III. List of magic wavelengths in Li, Na, and K atoms for the linearly polarized light.

	$np_{1/2} \rightarrow ns$		$np_{3/2} \rightarrow ns$			
	$\lvert 1/2\rvert$		$\lvert 1/2\rvert$		$\lvert 3/2\rvert$	
$m_j \rightarrow$	Present study	Ref. [26]	Present study	Ref. [26]	Present study	Ref. [26]
			Li			
$\alpha(\lambda_{\text{magic}})$	−328	−327.1(3)	−357	−357.26(7)	−288	−288.0(3)
λ_{magic}	550(1)	549.42(6)	557(1)	557.16(2)	537(3)	537.61(7)
$\alpha(\lambda_{\text{magic}})$	−398	398.7(2)	339	339.9(2)		
λ_{magic}	873(2)	872.57(9)	931(2)	930.3(2)		
$\alpha(\lambda_{\text{magic}})$	398.7(2)	339.9(2)				
λ_{magic}	872.57(9)	930.3(2)				
	$np_{1/2} \rightarrow ns$		$np_{3/2} \rightarrow ns$			
	$\lvert 1/2\rvert$		$\lvert 1/2\rvert$		$\lvert 3/2\rvert$	
$m_j \rightarrow$	Present study	Ref. [11]	Present study	Ref. [11]	Present study	Ref. [11]
Na						
$\alpha(\lambda_{\text{magic}})$	−520	−514(1)	−522	−517(1)		
λ_{magic}	514.73(1)	514.72(1)	515.01(1)	515.01(1)		
$\alpha(\lambda_{\text{magic}})$	−1981	−1956(3)	−2063	−2038(3)	−2002	−1976(3)
λ_{magic}	566.594(5)	566.57(1)	567.451(3)	567.43(1)	566.819(2)	566.79(1)
$\alpha(\lambda_{\text{magic}})$	53361	52760(100)	−66978	−66230(80)	−47	−42(2)
λ_{magic}	589.4570(1)	589.457	589.6363(1)	589.636	589.5563(3)	589.557(1)
$\alpha(\lambda_{\text{magic}})$	1931	1909(2)	1876	1854(2)		
λ_{magic}	615.872(1)	615.88(1)	616.708(1)	616.712(1)		
$\alpha(\lambda_{\text{magic}})$	244	241(1)	255	252(1)		
λ_{magic}	1028.6(4)	1028.7(2)	984.7(9)	984.8(1)		
			K			
$\alpha(\lambda_{\text{magic}})$	−208		−209		−210	
λ_{magic}	502.59(1)		503.70(2)		504.0(1)	
$\alpha(\lambda_{\text{magic}})$	−216		−218			
λ_{magic}	508.086(4)		509.31(5)			
$\alpha(\lambda_{\text{magic}})$	−218		−221		−221	
λ_{magic}	509.428(8)		510.83(2)		510.80(8)	
$\alpha(\lambda_{\text{magic}})$	−258		−260			
λ_{magic}	532(2)		533.07(1)			
$\alpha(\lambda_{\text{magic}})$	−262		−266		−265	
λ_{magic}	534.091(2)		535.81(2)		535.53(1)	
$\alpha(\lambda_{\text{magic}})$	−367		−371			
λ_{magic}	577.36(1)		578.71(8)			
$\alpha(\lambda_{\text{magic}})$	−379		−385		−384	
λ_{magic}	581.163(1)		583.168(1)		582.98(3)	
$\alpha(\lambda_{\text{magic}})$	−1203	−1186(2)				
λ_{magic}	690.137(2)	690.15(1)				
$\alpha(\lambda_{\text{magic}})$	−1272		−1243	−1226(3)	−1331	
λ_{magic}	693.775(1)		692.31(2)	692.32(2)	696.582(1)	
$\alpha(\lambda_{\text{magic}})$	21290	20990(80)	−27566	−27190(60)	−356	−356(8)
λ_{magic}	768.413(1)	768.413(4)	769.432(1)	769.432(2)	768.980(1)	768.980(3)
$\alpha(\lambda_{\text{magic}})$	479	472(1)	479	472(1)		
λ_{magic}	1227.73(1)	1227.7(2)	1227.73(2)	1227.7(2)		

trend as the right-handed circularly polarized light due to the linear dependency of the degree of polarizability $\mathcal{A}$ in Eq. (3).

In Table IV, we list magic wavelengths for the ns-$np_{1/2,3/2}$ transitions of Li, Na, and K atoms in the wavelength range 500–1500 nm in the presence of circularly polarized light. The number of magic wavelengths for the ns-$np_{1/2}$ transitions for the circularly polarized light are fewer compared to the linearly polarized light. Therefore, using the linearly polarized light to trap the atoms for these transitions would be more advantageous. However, the reported magic wavelengths could be useful in a situation that requires us to trap the atoms using circularly polarized light. Below, we discuss the results only for the ns-$np_{3/2}$ transitions as they seem to be of more experimental relevance owing to the fact that there are fewer convenient magic wavelengths for these transitions found using the linearly polarized light.

First, we discuss the results for the $2s$-$2p_{3/2}$ transition of a Li atom. As seen in Table IV, the number of convenient

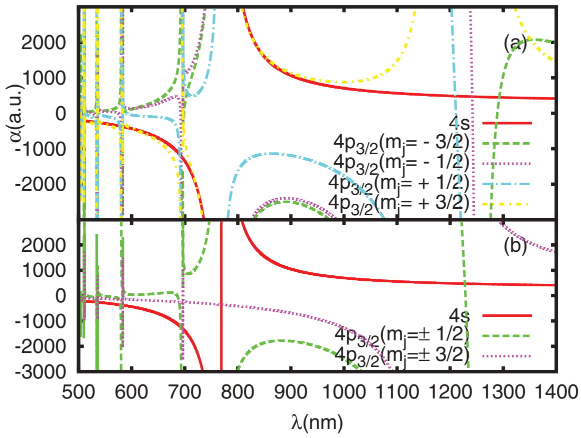

FIG. 6. (Color online) Total dynamic polarizability for $4s$ and $4p_{3/2}$ states of a K atom due to (a) linearly polarized light and (b) circularly polarized light. The magic wavelength for the corresponding $4s$-$4p_{3/2}$ transition is given by the crossing of two polarizability curves.

magic wavelengths for the above transition in this atom is fewer compared to linearly polarized light. Moreover, no magic wavelength was located for the $m_j = 3/2$ sublevel. Therefore, it would be appropriate to use linearly polarized light for the state-insensitive trapping of this atom. Next, we list a number of λ_{magic} and the corresponding polarizabilities for the $3s$-$3p_{3/2}$ transition of Na in the wavelength range 500–1500 nm in the same table. The number inside the brackets for λ_{magic} depicts the uncertainty of the match of polarizability curves for the two states involved in the transition. These uncertainties are found as the maximum differences between the $\alpha_{3s} \pm \delta\alpha_{3s}$ and $\alpha_{3p} \pm \delta\alpha_{3p}$ contributions with their respective magnetic quantum numbers, where $\delta\alpha$ are the uncertainties in the polarizabilities for their corresponding states. For a Na atom, we get a set of four magic wavelengths in between six $3p_{3/2}$ resonances lying in the wavelength range 500–1400 nm, i.e., the $3p_{3/2}$-$4s$ resonance at 1140.7 nm, the $3p_{3/2}$-$3d_j$ resonance at 819.7 nm, the $3p_{3/2}$-$5s$ resonance at 616.3 nm, the $3p_{3/2}$-$3s$ resonance at 589.2 nm, the $5p_{3/2}$-$4d_j$ resonance at 569 nm, and the $5p_{3/2}$-$6s$ resonance at 515.5 nm. The magic wavelength expected between the $3p_{3/2}$-$5s$ and $3p_{3/2}$-$3s$ resonances is

TABLE IV. List of magic wavelengths for the circularly polarized light in Li, Na, and K atoms.

	$np_{1/2} \to ns$		$np_{3/2} \to ns$			
$m_j \to$	$-1/2$	$1/2$	$-3/2$	$-1/2$	$1/2$	$3/2$
			Li			
$\alpha(\lambda_{\text{magic}})$	-274		-239	-316	-449	
λ_{magic}	533(1)		518.8(2.5)	546.1(1.3)	575.5(0.9)	
$\alpha(\lambda_{\text{magic}})$	596		779	432	250	
λ_{magic}	786.9(3)		754.2(3)	850.0(9)	1140(5)	
			Na			
$\alpha(\lambda_{\text{magic}})$	-522	-506	-530	-523	-517	
λ_{magic}	515.231(2)	513.25(6)	516.10(1)	515.28(1)	514.60(2)	
$\alpha(\lambda_{\text{magic}})$	-1884		-1893	-1991	-2076	
λ_{magic}	565.864(5)		565.963(7)	567.076(4)	567.947(3)	
$\alpha(\lambda_{\text{magic}})$	1994	1863	1974	1923	1878	
λ_{magic}	615.412(1)	617.352(7)	615.694(1)	616.435(1)	617.117(2)	
$\alpha(\lambda_{\text{magic}})$	211			237	283	
λ_{magic}	1252.9(8)			1061.7(3)	909.2(4)	
			K			
$\alpha(\lambda_{\text{magic}})$		-205		-208	-208	-210
λ_{magic}		501.68(5)		503.83(3)	503.48(5)	505.0(2)
$\alpha(\lambda_{\text{magic}})$		-212		-218	-216	
λ_{magic}		506.17(6)		509.73(1)	508.71(2)	
$\alpha(\lambda_{\text{magic}})$	-218	-217	-219.39	-219.26	-219.30	-219.26
λ_{magic}	509.9(8)	509.57(2)	$-510.90(4)$	510.82(3)	510.84(2)	510.85(3))
$\alpha(\lambda_{\text{magic}})$			-219.8	-219.9	-220.0	-220.5
λ_{magic}			511.168(1)	511.20(8)	511.298(4)	511.56(3)
$\alpha(\lambda_{\text{magic}})$	-259	-250		-259	-257	-265
λ_{magic}	533.5(5)	528.74(8)		534(3)	532.21(3)	536.66(2)
$\alpha(\lambda_{\text{magic}})$	-374	-348		-370	-363	-382
λ_{magic}	579(2)	572.02(7)		579.645(3)	577.25(2)	583.598(2)
$\alpha(\lambda_{\text{magic}})$	-1169	-1170				
λ_{magic}	690.072(2)	690.137(2)				
$\alpha(\lambda_{\text{magic}})$	-1205	-1069	-1292	-1228	-1179	-1294
λ_{magic}	692.104(1)	683.83(2)	696.60976(1)	693.329(1)	690.63(6)	696.69199(1)
$\alpha(\lambda_{\text{magic}})$	468		453	475	491	
λ_{magic}	1255.37(4)		1292.7(2)	1241.6(1)	1209.4(9)	

TABLE V. List of average magic wavelengths λ_{magic}(avg) for Li, Na, and K atoms for the linearly polarized light.

Atom	$np_{1/2} \rightarrow ns$	$np_{3/2} \rightarrow ns$
Li	550(1)	547(20)
	873(2)	931(2)
Na	514.73(1)	515.01(1)
	566.59(1)	567(1)
	589.4570(1)	589.6(1)
	616.872(1)	616.708(1)
	1028.6(4)	984.7(9)
K	502.59(1)	503.8(3)
	508.086(4)	509.31(5)
	509.43(1)	10.8(1)
	532(2)	533.07(1)
	534.091(2)	535.7(3)
	577.36(1)	578.7(1)
	581.163(1)	583.1(8)
	690.137(2)	
	693.7752(1)	694(4)
	768.413(1)	768.6(5)
	1227.73(1)	1227.73(2)

TABLE VI. List of average magic wavelengths λ_{magic}(avg) for Li, Na, and K atoms for left-circularly polarized light.

Atom	$np_{1/2} \rightarrow ns$	$np_{3/2} \rightarrow ns$
Li	533(1)	
	786.9(3)	
Na	514(2)	515(2)
	565.86(1)	567(2)
	616(2)	616(1)
	1252.9(8)	985(153)
K	501.7(1)	504(1)
	506.2(1)	509(1)
	509.7(3)	510.9(1)
		511.3(4)
	531(5)	534(4)
	576(7)	580(6)
	690.1(1)	
	688(4)	694(6)
	1255.37(4)	1248(84)

missing for the circularly polarized traps. Half of the magic wavelengths support blue-detuned optical traps whereas the other half favor the red-detuned optical traps. It can be observed from Table IV that the $m_j = 3/2$ sublevel does not support state-insensitive trapping at any of the listed magic wavelengths. However, using a switching trapping scheme as described in [12] can allow trapping this sublevel too. The magic wavelength at 616 nm is recommended owing to the fact that it supports a strong red-detuned trap, as depicted by a large positive value of polarizability at this wavelength. For the $4s$-$4p_{3/2}$ transition in a K atom, we get eight sets of magic wavelengths in the wavelength range 500–1500 nm, as shown in Table IV. Out of these eight magic wavelengths, the magic wavelength at 1247 nm supports red-detuned optical traps. The magic wavelengths at 510.9, 511.3, and 694 nm occur for all the m_j sublevels at nearly same value of polarizability. However, at 511.3 and 694 nm the crossing for polarizability curves for the $4s$ and $4p_{3/2}$ states is very sharp. In addition to the magic wavelengths mentioned in Table IV, we found five more magic wavelengths for the $m_j = 3/2$ state at 516.8(7), 543.4(5), 605.2(9), 724.5(3), and 849.7(8) nm.

The final magic wavelengths are calculated as the average of the magic wavelengths for various m_j sublevels and are written as λ_{magic}(avg) in Tables V and VI for linearly and circularly polarized light, respectively. The error in the λ_{magic}(avg) is calculated as the maximum difference between the magic wavelengths from different m_j sublevels. For cases where the magic wavelength was found for only one m_j sublevel (for example, λ_{magic} for the $4s$-$4p_{3/2}$ transition at 1227.73 nm for K atoms), the number in the parentheses corresponds to the uncertainty in the match of the polarizabilities of the ns and np states in place of representing the spread in the magic wavelengths for various m_j sublevels.

V. SUMMARY

In summary, we have investigated magic wavelengths in Li, Na, and K atoms for both the linearly and circularly polarized optical traps. To determine these values, we have calculated dynamic polarizabilities using the best known $E1$ matrix elements. Our predictions for the linearly polarized trap agree well with the previously reported results. This study demonstrates a significant number of magic wavelengths due to the the circularly polarized light which will be very useful in trapping the above atoms in the ac-Stark-shift-free regime. However, we do not recommend using the circularly polarized traps for trapping Li atoms.

ACKNOWLEDGMENTS

The work of B.A. was supported by the University Grants Commission and the Department of Science and Technology, India. Computations were carried out using the 3TFLOP HPC Cluster at the Physical Research Laboratory, Ahmedabad.

---

[1] A. Kazantsev, G. Surdutovich, and V. Yakovlev, *Mechanical Action of Light on Atoms* (World Scientific, Singapore, 1990).

[2] R. Grimm, M. Weidemller, and Yu. B. Ovchinnikov, Adv. At. Mol. Opt. Phys. **42**, 95 (2000).

[3] V. Balykin, V. Minogin, and V. Letokhov, Rep. Prog. Phys. **63**, 1429 (2000).

[4] M. S. Safronova, C. J. Williams, and C. W. Clark, Phys. Rev. A **67**, 040303(R) (2003).

[5] M. Takamoto and H. Katori, Phys. Rev. Lett. **91**, 223001 (2003).

[6] H. Katori, T. Ido, and M. Kuwata-Gonokami, J. Phys. Soc. Jpn. **68**, 2479 (1999).

[7] H. Katori, in *Proceedings of the Sixth Symposium on Frequency Standards and Metrology*, edited by P. Gill (World Scientific, Singapore, 2002), pp. 323–330.

[8] C. A. Sackett, D. Kielpinski, B. E. King, C. Langer, V. Meyer, C. J. Myatt, M. Rowe, Q. A. Turchette, W. M. Itano, D. J. Wineland *et al.*, Nature (London) **404**, 256 (2000).

[9] A. D. Ludlow *et al.*, Science **319**, 1805 (2008).

[10] J. McKeever, J. R. Buck, A. D. Boozer, A. Kuzmich, H.-C. Nagerl, D. M. Stamper-Kurn, and H. J. Kimble, Phys. Rev. Lett. **90**, 133602 (2003).

[11] B. Arora, M. S. Safronova, and C. W. Clark, Phys. Rev. A **76**, 052509 (2007).

[12] B. Arora and B. K. Sahoo, Phys. Rev. A **86**, 033416 (2012).

[13] V. V. Flambaum, V. A. Dzuba, and A. Derevianko, Phys. Rev. Lett. **101**, 220801 (2008).

[14] C. Y. Park, H. Noh, C. M. Lee, and D. Cho, Phys. Rev. A **63**, 032512 (2001).

[15] N. L. Manakov, V. D. Ovsiannikov, and L. P. Rapoport, Phys. Rep. **141**, 319 (1986).

[16] B. Arora, D. Nandy, and B. K. Sahoo, Phys. Rev. A **85**, 012506 (2012).

[17] I. Lindgren, Int. J. Quantum Chem. Symp. **12**, 33 (1978).

[18] B. K. Sahoo, B. P. Das, and D. Mukherjee, Phys. Rev. A **79**, 052511 (2009).

[19] D. Mukherjee, B. K. Sahoo, H. S. Nataraj, and B. P. Das, J. Phys. Chem. A **113**, 12549 (2009).

[20] B. K. Sahoo, S. Majumder, R. K. Chaudhuri, B. P. Das, and D. Mukhrejee, J. Phys. B **37**, 3409 (2004).

[21] D. K. Nandy, Y. Singh, B. P. Shah, and B. K. Sahoo, Phys. Rev. A **86**, 052517 (2012).

[22] U. Volz and H. Schmoranzer, Phys. Scr. T **65**, 48 (1996).

[23] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. Ref. Data Ser. Vol. 35 (U.S. Government Printing Office, Washington, D.C., 1971).

[24] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team. NIST Atomic Spectra Database (version 5.0), http://physics.nist.gov/asd.

[25] J. Sansonetti, W. Martin, and S. Young, Handbook of basic atomic spectroscopic data, version 1.1.2, http://physics.nist.gov/Handbook.

[26] M. S. Safronova, U. I. Safronova, and C. W. Clark, Phys. Rev. A **86**, 042505 (2012).

[27] A. Miffre, M. Jacquest, M. Buchner, G. Trenec, and J. Vigue, Eur. Phys. J. D **38**, 353 (2006).

[28] A. Derevianko, W. R. Johnson, M. S. Safronova, and J. F. Babb, Phys. Rev. Lett. **82**, 3589 (1999).

[29] C. R. Ekstrom, J. Schmiedmayer, M. S. Chapman, T. D. Hammond, and D. E. Pritchard, Phys. Rev. A **51**, 3883 (1995).

[30] L. Windholz and M. Musso, Phys. Rev. A **39**, 2472 (1989).

[31] W. F. Holmgren, M. C. Revelle, V. P. A. Lonij, and A. D. Cronin, Phys. Rev. A **81**, 053607 (2010).

[32] K. E. Miller, D. Krause, and L. R. Hunter, Phys. Rev. A **49**, 5128 (1994).

[33] C. Krenn, W. Scherf, O. Khait, M. Musso, and L. Windholz, Z. Phys. D **41**, 229 (1997).