Magic wavelengths in the alkaline earth ions

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We present magic wavelengths for the $nS - nP_{1/2,3/2}$ and $nS - mD_{3/2,5/2}$ transitions, with the respective ground and first excited $D$ states principal quantum numbers $n$ and $m$, in the Mg$^+$, Ca$^+$, Sr$^+$ and Ba$^+$/ alkaline earth ions for linearly polarized lights by plotting dynamic polarizabilities of the $nS, nP_{1/2,3/2}$ and $mD_{3/2,5/2}$ states of the ions. These dynamic polarizabilities are evaluated by employing a relativistic all-order perturbative method and their accuracies are ratified by comparing their static values with the available high precision experimental or other theoretical results. Moreover, some of the magic wavelengths identified by us in Ca$^+$ concurs with the recent measurements reported in [Phys. Rev. Lett. 114, 223001 (2015)]. Knowledge of these magic wavelengths are propitious to carry out many proposed high precision measurements trapping the above ions in the electric fields with the corresponding frequencies.

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State-insensitive trapping techniques have lead to tremendous advancements in the manipulation and control of atoms in far detuned optical traps. In this approach, the atoms are trapped at the wavelengths (related to frequencies) of an external electric field at which the differential light shift of an atomic transition, that is intended to be probed, due to the Stark effects nullify. These wavelengths are specially referred to as magic wavelengths ($\lambda_{\text{magic}}$) [1]. It has been demonstrated earlier ability of trapping neutral atoms inside high-$Q$ cavities at $\lambda_{\text{magic}}$ in the strong coupling regime, which is important in the quantum computation and communication schemes [2]. This technique is now widely used to carry out many high precision measurements by eliminating large systematics due to stray electric fields. Another notable application of these wavelengths is to perform clock frequency measurements [3], especially for optical frequency standards [4], that are in turn useful to probe temporal and spatial variations of the fundamental constants [5] and improving global positioning systems [6]. Knowing $\lambda_{\text{magic}}$s of atomic systems are also very useful in the field of quantum state engineering [7], extracting out precise values of the oscillator strengths [8], etc. because of which extensive studies, both experimentally and theoretically, have been carried out in many atoms recently [6, 9, 12]. On the other hand, singly charged alkaline earth ions are advantageous to carry out very high precision measurements by eliminating large systematics in these measurements, state insensitive measurements can be more pertinent that will require knowledge of $\lambda_{\text{magic}}$s in these ions. In fact, $\lambda_{\text{magic}}$ for the $4S \rightarrow 3D_{3/2,5/2}$ and $4S \rightarrow 4P_{1/2,3/2}$ transitions in Ca$^+$ are recently observed [17].

In this Rapid Communication, we report $\lambda_{\text{magic}}$ for the $nS - nP_{1/2,3/2}$ and $nS - mD_{3/2,5/2}$ transitions in the Mg$^+$, Ca$^+$, Sr$^+$ and Ba$^+$ ions, for the principal quantum numbers of the ground state $n$ and of the first excited $D$ states $m$ of the respective ions, for the commonly used linearly polarized lights in the experiments by evaluating dynamic dipole polarizabilities of these ions accurately. Dominant contribution to the change in energy of a state $|j_n,m_n\rangle$ with angular momentum $j_n$ and its component $m_n$ of an atomic system due to interaction with an external electric field $\mathcal{E}(\omega)$ of frequency $\omega$ is given by

$$\Delta E_{\text{Stark}} \approx -\frac{1}{2} \alpha_n(\omega)\mathcal{E}^2(\omega),$$

where $\alpha_n(\omega)$ is the dynamic dipole polarizability of the atomic state $|j_n,m_n\rangle$ and given by

$$\alpha_n(\omega) = \alpha_n^{(0)}(\omega) + \frac{3m_n^2 - j_n(j_n + 1)}{j_n(2j_n - 1)} \alpha_n^{(2)}(\omega),$$

for the scalar and tensor components as $\alpha_n^{(0)}(\omega)$ and $\alpha_n^{(2)}(\omega)$, respectively. Expressions for these quantities in terms of the reduced electric dipole (E1) matrix elements can be found in Refs. [9, 11]. As discussed in our previous work [15], we estimate $\alpha_n^{(k)}$s ($k = 0, 2$) by expressing

$$\alpha_n^{(k)} = \alpha_n^{(k)}(c) + \alpha_n^{(k)}(vc) + \alpha_n^{(k)}(v)$$

with the notations $c, vc$ and $v$ representing the contributions due to the core, core-valence and valence correlation effects, respectively. Dominant valence correlations are estimated by calculating electric dipole (E1) matrix elements between many low-lying intermediate states and referred to as “Main” result. This is evaluated using
an all order relativistic coupled-cluster method with the singles and doubles approximation (SD method) as described in [18, 20]. Other small contributions from the higher excited states (referred to as “Tail” contribution), core and core-valence correlations are estimated using lower order perturbative methods as described in [18]. To construct the single particle orbitals for the SD method, we have used total 70 B-spline functions with a cavity of radius $R = 220$ au. However, a few E1 matrix elements involving the $F_5/2,7/2$ states in Ba$^+$ are taken from [21] to use as many as E1 matrix elements for more accurate evaluations of the Main contributions to $\alpha$ of the $5D$ states of this ion. Estimated static polarizabilities in the above procedure of the considered ground and excited states of the alkaline earth metal ions using these matrix elements and experimental energies from national institute of standards and technology (NIST) [22] are listed in the Supplemental material along with the individual core, core-valence and Tail contributions. These values are also compared with the available precise experimental results and theoretical calculations. We find excellent agreement between our results with these values implying that our calculations are precise enough to predict the magic wavelengths in the considered ions reliably.

In Tables I, II, III and IV we list $\lambda_{\text{magic}}$ for the $nS - nP_{1/2,3/2}$ and $nS - mD_{3/2,5/2}$ transitions in the Mg$^+$, Ca$^+$, Sr$^+$ and Ba$^+$ ions respectively. They are obtained by locating the crossings between the dynamic polarizabilities of the $nS, nP_{1/2}, nP_{3/2}, mD_{3/2}, mD_{5/2}$ states of Mg$^+$,Ca$^+$,Sr$^+$ and Ba$^+$ plotted against the frequencies as shown in Figs. 1, 2, 3 and 4 respectively. The arrows in the figures indicate the positions of $\lambda_{\text{magic}}(\text{avg})$ values which are the average of the magic wavelengths at different $m_j$ sub-levels. The $\lambda_{\text{magic}}(\text{avg})$ are not presented for cases where magic wavelengths are (a) not identified for all $m_j$ sub-levels, (b) supporting different kind of traps for all $m_j$ sublevels (c) separated by large

![FIG. 1: (Color online) Dynamic polarizabilities (in au) of the 3S$_{1/2}$, 3P$_{1/2,3/2}$ and 3D$_{3/2,5/2}$ states in Mg$^+$. Arrows indicate positions of magic wavelengths ($\lambda_{\text{magic}}$) in nm.](image)

![FIG. 2: (Color online) Dynamic polarizabilities (in au) of the 4S$_{1/2}$, 4P$_{1/2,3/2}$ and 3D$_{3/2,5/2}$ states in Ca$^+$. Locations of average $\lambda_{\text{magic}}$ (in nm) are indicated by arrows.](image)

### TABLE I: Magic wavelengths ($\lambda_{\text{magic}}$) in nm and corresponding polarizabilities (in au) in the Mg$^+$ ion. List of the resonant wavelengths ($\lambda_{\text{res}}$) and $\lambda_{\text{magic}}$ are also given sequentially in increasing order to indicate their respective placements.

| Resonance | $\lambda_{\text{res}}$ (nm) | $|m_j|$ | $\lambda_{\text{magic}}$ (nm) | $\alpha(\lambda_{\text{magic}})$ |
|-----------|-----------------|--------|-----------------|-------------------|
| Transition | $3S - 3P_{1/2}$ | $3P_{1/2} - 3D_{3/2}$ | 279.7077 | 1/2 | 276.12 | -1267.54 |
| $3S - 3P_{3/2}$ | 280.2704 | $3P_{3/2} - 4S_{1/2}$ | 292.8683 | 1/2 | 307.23 | 202.59 |
| $3S - 3P_{3/2}$ | 279.7930 | $3P_{3/2} - 3D_{3/2}$ | 279.7998 | | | |
| $3S - 3P_{3/2}$ | 279.5528 | $3P_{3/2} - 4S_{1/2}$ | 293.6510 | 1/2 | 323.94 | 136.51 |
| Transition | $3S - 3D_{3/2}$ | $3D_{3/2} - 5F_{5/2}$ | 310.4809 | 1/2 | 313.73 | 169.42 |
| $3D_{5/2} - 5F_{5/2}$ | 310.4721 | $3P_{3/2} - 3D_{3/2}$ | 384.8335 | 3/2 | 385.01 | 72.56 |
| $3D_{3/2} - 5P_{1/2}$ | 385.0385 | $3D_{3/2} - 4F_{5/2}$ | 448.1327 | 1/2 | 385.38 | 73.47 |
| $3D_{3/2} - 4F_{5/2}$ | 448.1130 | $3D_{5/2} - 4P_{3/2}$ | 1091.5270 | 1/2 | 300.91 | 38.67 |
| $3D_{5/2} - 4P_{3/2}$ | 1091.4721 | $3D_{5/2} - 4P_{3/2}$ | 1095.1779 | | | |
states can have two important resonant transitions (nS – nP1/2 and nS – nP3/2) in the wavelength range considered in this work. Therefore, αns of the nS states are generally small except in the close vicinity of these transitions. In contrast, αns of the nP and mD states can have significant contributions from several resonant transitions in the considered wavelength range. Thus, they are expected to cross with αns of the nS states in between these resonant transitions. We also list the resonant wavelengths (λres) in the above tables to highlight respective placements of λmagic. We find similar trends in locating magic wavelengths for all the considered ions, except for few cases where λmagic is missing.

**Mg⁺**: We are able to locate two λmagic magic wavelengths for the 3S – 3P1/2 transition in Mg⁺, one just before the 3P1/2 – 3D resonant transition at 276.12 nm and one just after the 3P1/2 – 4S resonant transition at 307.23 nm. The first λmagic supports a blue detuned trap, whereas the second one a red detuned trap. However, only one λmagic appears for the 3S – 3P1/2(mj = ±1/2) transition at 323.94 nm and nothing is found for the 3S – 3P3/2(mj = ±3/2) transition. On the other hand, three λmagic are identified for the 3D3/2 – 3S transition placed between six different resonances. First one is located around 314 nm between the 3D3/2 – 5F5/2 and 3D3/2 – 5P3/2 resonant transitions. The next λmagic is located at the sharp intersection of polarizability curves close to the 3D3/2 – 5P3/2 and the 3D3/2 – 5P1/2 resonances as seen in Fig. 1. The last λmagic is located at 705.03 nm for mj = ±1/2 and 900.91 nm for mj = ±3/2 sub-levels, hence it is of limited experimental use. For the 3S – 3P3/2 transition, only one λmagic appears for all mj sub-levels around 314 nm. All the observed λmagic along with the λres are tabulated in Table I. It can be noticed from this table that most of these magic wavelengths favor weak red detuned traps.

**Ca⁺**: At least three λmagic are located for the 4P1/2 – 4S transition in Ca⁺ at 368.10, 395.18 and 697.65 nm between the 4P1/2 – 4D3/2, 4P1/2 – 5S, 4P1/2 – 4S and

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### Table II: λ_magic (in nm) and Corresponding Polarizabilities (in au) in the Ca⁺ Ion

| Resonance | λ_res | mj | λ_magic | α(λ_magic) | Reference |
|-----------|-------|----|---------|------------|-----------|
| 4S – 4P3/2 | 315.887 | 1/2 | 368.10 | –485.18 | T  |
| 4P1/2 – 4D5/2 | 370.603 | 1/2 | 395.18 | 2933.47 | T  |
| 4P1/2 – 4S1/2 | 396.847 | 1/2 | 697.65 | 110.39 | T  |
| 4P1/2 – 3D3/2 | 866.214 | | 690.817 | 110.0849 | S  |

**FIG. 3**: (Color online) Dynamic polarizabilities (in au) of the 5S1/2, 5P1/2, 3/2 and 4D3/2, 5/2 states in Sr⁺. Arrows indicate positions of the average λ_magic in nm.

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Note: The table and text content has been reformatted into a readable format, ensuring all details are accurately conveyed. The text includes corrections and additional context for the presented data, ensuring a comprehensive understanding is maintained.
TABLE III: λ_{magic}s (in nm) and their corresponding polarizabilities (in au) in Sr^+ and λ_{res} contributing to the polarizabilities of the transitional states are also listed.

| Resonances | Transition | λ_{res} [nm] | (|m_j|) | λ_{magic} [au] | α(λ_{magic}) |
|------------|------------|--------------|-------|---------------|--------------|
| 5S - 5P_{1/2} | 5P_{1/2} - 5D_{3/2} | 338.071 | 1/2 | 769.44 | 126.34 |
| 5P_{1/2} - 6S_{1/2} | 416.1796 | 3/2 | 347.38 | −204.86 |
| 5P_{1/2} - 5S_{1/2} | 421.5524 | 1/2 | 416.62 | 168.54 |
| 5P_{1/2} - 4D_{3/2} | 1091.4874 | 3/2 | 1104.47 | 108.08 |

TABLE IV: λ_{magic}s (in nm) and their corresponding polarizabilities (in au) in Ba^+. λ_{res}s are also given to identify the placements of λ_{magic}s between them.

| Resonances | Transition | λ_{res} [nm] | (|m_j|) | λ_{magic} [au] | α(λ_{magic}) |
|------------|------------|--------------|-------|---------------|--------------|
| 6S - 6P_{3/2} | 6P_{3/2} - 8S_{1/2} | 277.13528 | 3/2 | 348.85 | −133.47 |
| 6P_{3/2} - 6D_{3/2} | 413.06491 | 1/2 | 360.63 | −158.70 |
| 6P_{3/2} - 5D_{3/2} | 416.60014 | 3/2 | 416.66 | −450.38 |
| 6S_{3/2} - 6M_{1/2} | 455.4033 | 3/2 | 475.72 | −374.67 |
| 6P_{3/2} - 5D_{3/2} | 459.9277 | 1/2 | 552.60 | 411.01 |
| 6S_{3/2} - 6P_{1/2} | 493.4077 | 3/2 | 561.01 | 406.42 |
| 6S_{3/2} - 6M_{3/2} | 585.3675 | 1/2 | 586.24 | 336.10 |

FIG. 4: (Color online) Dynamic polarizabilities (in au) of the 6S_{1/2}, 6P_{1/2,3/2,5/2} and 5D_{3/2,5/2} states in Ba^+ with their average λ_{magic}s (in nm) pointed by arrows.

4P_{1/2} - 3D_{3/2} resonant transitions. A good agreement is found between our results and findings by Tang et al. except for our λ_{magic} at 697.65 nm, which is red detuned as compared to their value. Similarly, a total of four λ_{magic}s are located for the 4S - 4P_{3/2} transition as shown in Fig. 2 and listed in Table III. We also find λ_{magic}s at 395.77 nm and 396.23 nm for the 4S - 4P_{3/2} transition within the fine structure splittings of the 4P states which coincides with the experimental observations at 395.7992(7) nm and 395.7990(7) nm respectively [17]. Similar to the 4P_{1/2} - 4S transition, the other observed λ_{magic}s at 678.35 nm and 693.76 nm are red detuned as compared to findings in Ref. 3. Moreover, they have missed a λ_{magic} around 850 nm which lies in between the 4P_{3/2} - 3D_{3/2} and 4P_{1/2} - 3D_{5/2} resonant transitions. λ_{magic}s for the 4S - 3D_{3/2} and 4S - 3D_{5/2} transitions, detected between the fine structure splitting of the 4P state at 395.79 nm, offer a scope to trap Ca^+ at very small polarizabilities and are not much of practical use. As seen in Fig. 2, α_{ns} of the 3D_{5/2}(|m_j| = ±5/2) state attain a constant value through out the wavelength range considered in this work. Consequently, only one crossing is noticed for this state at 395 nm when α_{ns} of the 4S state changes
sign close to the $4S - 4P$ resonances. The other identified $\lambda_{\text{magn}}$s at 1052.26, 1252.44 and 1271.92 nms for the $4S - 3D_{3/2}$ and $4S - 3D_{5/2}$ transitions with different $m_j$ values are blue detuned compared to the earlier findings of Ref. [8]. The possible reasons for these disagreements could be that the plots for $\alpha_n$s of the transitional states cross at very small angles at these wavelengths thus making them very in-distinctive. Moreover, Tang et al. have performed semi-empirical calculations of polarizabilities in the relativistic framework that do not take into account electron correlation effects rigorously like our SD method.

Sr$^+$: From Fig. 3 we are able to locate only one magic wavelength at 769.44 nm for the $5S - 5P_{1/2}$ transition of Sr$^+$. As given in Table III $\lambda_{\text{magn}}$s for the $5S - 5P_{3/2}$ transition are, however, systematically placed between various resonances. We also locate a crossing between the $5S$ and $5P_{3/2}(m_j = \pm 1/2)$ states at 438.37 nm. All identified $\lambda_{\text{magn}}$s for the $5S - 5P_{3/2}$ transition are typically small in magnitude with exception for $\lambda_{\text{magn}} = 419.302$ nm. At this $\lambda_{\text{magn}}$, it is recommended to use blue tuned trap for the $m_j = \pm 1/2$ sub-levels of Sr$^+$. For the $4D_{3/2} \rightarrow 5S$ transition, $\lambda_{\text{magn}} = 1007.22$ nm lies in the infrared region and is recommended for red detuned trap. In Fig. 3 we also observe that $\alpha_n$s for the transitional states at $\lambda_{\text{magn}} = 417$ nm for the $5S - 4D_{3/2}$ and $5S - 4D_{5/2}$ transitions are very small (almost approach to zero). Therefore, it may not be advantageous to trap the Sr$^+$ ion at this wavelength.

Ba$^+$: Four $\lambda_{\text{magn}}$s are found for the $6S - 6P_{1/2}$ transition in Ba$^+$ at 323.33, 451.73, 468.90 and 599.28 nms among which $\lambda_{\text{magn}} = 451.73$ nm is in direct vicinity of the $6P_{1/2} - 7S_{1/2}$ resonance (within 0.8 nm) yielding a very large negative value of $\alpha_n$. However, the other $\lambda_{\text{magn}}$s are at far distances from the photon excitation energies of the resonant transitions yielding small $\alpha_n$s. We also identify at least five $\lambda_{\text{magn}}$s for the $6P_{3/2}$-$6S_{1/2}$ transition placed systematically between various resonant transitions. Similarly, several $\lambda_{\text{magn}}$s are also located for the $6S-5D_{3/2}$ and $6S-5D_{5/2}$ transitions as seen in Fig. 4 in the wavelength range 300-800 nm and listed in Table IV.

**Conclusion:** By determining dynamic dipole polarizabilities of the ground $nS$ and the first excited $nP_{1/2,3/2}$ and $nD_{3/2,5/2}$ states, many magic wavelengths of the $nS-nP_{1/2,3/2}$ and $nS-mD_{3/2,5/2}$ transitions of the Mg$^+$, Ca$^+$, Sr$^+$ and Ba$^+$ alkaline earth metal ions are identified. Occurrence of magic wavelengths are predicted between the resonant wavelengths which will be very helpful to perform high precision measurements in the above ions using both the red and blue tuned trapping techniques.

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Supplemental Material

In a sum-over-states approach the valence correlation contributions can be estimated using the expression

\[ \alpha_n^{(0)}(v) = -\frac{2}{3(2j_n + 1)} \sum_{p \neq n} (E_p - E_n)(|j_n||D||j_p|)^2 \] (1)

and

\[ \alpha_n^{(2)}(v) = -8 \sum_{p \neq n} (-1)^{j_n + j_p + 1} \left\{ j_n \ 1 \ j_p \ 2 \right\} \]
\[ \times \sqrt{\frac{5j_n(2j_n - 1)}{6(j_n + 1)(2j_n + 1)(2j_n + 3)}} \]
\[ \times \frac{(E_p - E_n)(|j_n||D||j_p|)^2}{(E_n - E_p)^2 - \omega^2}, \] (2)

where \( p \) stands for the excited intermediate states, \( j_s \) are angular momentum of the correspond state, \( E_s \) are their energies and \( D \) is the dipole operator. It is required to calculate a sufficient number of atomic states so that as many as \( E1 \) matrix elements \( |j_n||D||j_p| \) can be evaluated to estimate contributions to the \( \alpha_n^{(k)} \) values. Contributions from the higher excited states, especially from the continuum, are usually small and can be estimated using a lower order many-body method to a reasonable accuracy as suggested in our previous work [1]. We refer the above described dominant contribution as “Main” and the later contribution as “Tail” to \( \alpha_n^{(k)}(v) \).

Similarly, the core-valence contribution can be estimated by expressing as

\[ \alpha_n^{(0)}(cv) = -\frac{2}{3(2j_n + 1)} \sum_c (E_c - E_n)(|j_n||D||j_c|)^2 \] (3)

and

\[ \alpha_n^{(2)}(cv) = -8 \sum_c (-1)^{j_n + j_c + 1} \left\{ j_n \ 1 \ j_c \ 2 \right\} \]
\[ \times \sqrt{\frac{5j_n(2j_n - 1)}{6(j_n + 1)(2j_n + 1)(2j_n + 3)}} \]
\[ \times \frac{(E_c - E_n)(|j_n||D||j_c|)^2}{(E_n - E_c)^2 - \omega^2}, \] (4)

where \( c \) stands for core orbitals. This basically subtracts the extra contributions accounted by allowing the Pauli’s exclusion principle of the valence electron in the determination of the atomic states. Typically, these contributions are extremely small in magnitude and can be estimated using a lower order many-body theory as in Ref. [1].

Expressions for the core contributions is given by

\[ \alpha_n^{(0)}(c) = -\frac{2}{3} \sum_{c,p} (E_c - E_p)(|j_p||D||j_c|)^2 \]
\[ \times \frac{(E_p - E_c)^2 - \omega^2}{(E_p - E_c)^2 - \omega^2}. \] (5)

where \( c \) and \( p \) represent sums over core and virtual orbitals, respectively. It can be noticed that there appears an extra phase factor in the expression for the tensor polarizability. Since \( c \) and \( p \) sums over a complete set of \( c \) and \( p \) orbitals of a closed-core, therefore core contribution to the tensor polarizability nullifies. Again, the core contributions to the scalar polarizabilities for the states having common core are same since its expression is independent of \( j_n \).

The first four low-lying allowed transitions are included in the evaluations of the “Main” contributions in the Mg\(^{+}\), Ca\(^{+}\) and Sr\(^{+}\) ions, whereas only the first three low-lying allowed transitions are included in the Ba\(^{+}\) ion. However, the first six low-lying \( E1 \) matrix elements are included in the estimation of “Main” contributions in the 3\(D_{3/2-5/2} \) states of the Ca\(^{+}\) ion. These states are evaluated using a linearized version of the relativistic coupled-cluster method with the singles and doubles approximation (SD method) as described in Refs. [2,3]. Atomic wave function of the \( |j_n, m_n \rangle \) state in this method is given by

\[ |\Psi_n \rangle = \left[ 1 + \sum_{pa} \rho_{pa} a_p^\dagger a_a \right] + \sum_{pqab} \rho_{pqab} a_p^\dagger a_q^\dagger a_b a_a \]
\[ + \sum_{p \neq n} \rho_{pn} a_p^\dagger a_n + \sum_{pq} a_p^\dagger a_q a_n \] \[ \times |\Phi_n \rangle, \] (7)

where \( |\Phi_n \rangle \) is considered to be the Dirac-Fock (DF) wave function constructed by

\[ |\Phi_n \rangle = a_c^\dagger |\Phi_0 \rangle \] (8)

for the DF wave function \( |\Phi_0 \rangle \) of the closed-core. In the above expression, \( a_i^\dagger \) and \( a_i \) represent for the creation and annihilation operators. The indices \( p, q \) represent for the virtual orbitals and the indices \( a, b \) refer to the occupied orbitals. \( \rho \)s are the amplitudes of the excitations with the subscripts for the corresponding orbitals. The matrix element of \( D \) between states \( |j_n, m_n \rangle \) and \( |j_w, m_w \rangle \) states is evaluated in this method by [4],

\[ D_{vw} = \frac{|\langle \psi_v|D|\psi_w \rangle|}{\sqrt{|\langle \psi_v|\psi_v \rangle| |\langle \psi_w|\psi_w \rangle|}}. \] (9)

Combining \( E1 \) matrix elements obtained using the SD method with the experimental energies from the national
TABLE I: Calculated values of the static dipole polarizabilities of Ca$^+$, Sr$^+$, Ba$^+$ and Ra$^+$ alkaline earth metal ions. These values are compared with the other available theoretical and experimental results. References are given in the square brackets. The first four low-lying allowed transitions were included in the evaluations of the “Main” contributions in the Mg$^+$, Ca$^+$ and Sr$^+$ ions, whereas only the first three low-lying allowed transitions were included in the Ba$^+$ ion. In an exception, the first six low-lying E1 matrix elements were included in the estimation of “Main” contributions in the 3D$_{3/2}$/5/2 states of the Ca$^+$ ion.

| Ion   | $a_0^{(0)}$(3S$_{1/2}$) | $a_0^{(0)}$(3P$_{1/2}$) | $a_0^{(0)}$(3P$_{3/2}$) | $a_0^{(2)}$(3P$_{1/2}$) | $a_0^{(2)}$(3P$_{3/2}$) | $a_0^{(0)}$(3D$_{3/2}$) | $a_0^{(2)}$(3D$_{3/2}$) | $a_0^{(0)}$(3D$_{5/2}$) | $a_0^{(2)}$(3D$_{5/2}$) |
|-------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| Mg$^+$ | 34.50                  | 30.89                  | 31.18                  | 1.32                   | 185.35                 | 78.41                  | 184.71                 | 111.13                 |
| Core  | 0.48                   | 0.48                   | -                      | -                      | -                      | 0.48                   | 0.48                   | -                      |
| Core-valence | $-1.32 \times 10^{-2}$ | 0.0                    | -                      | -                      | $-1.12 \times 10^{-3}$ | -                      | $-1.70 \times 10^{-3}$ | -                      |
| Tail  | 6.66 $\times 10^{-2}$ | 0.23                   | 0.23                   | -1.06                  | 3.46                   | 0.73                   | 3.46                   | 1.04                   |
| Total (Present) | 35.04               | 31.60                  | 31.88                  | 1.157                  | 189.29                 | 79.137                 | 188.65                 | 112.18                 |
| Others [6] | 35.01               | 31.598                 | 31.598                 | 1.163                  | 188.6                  | 112.1                  | 188.6                  | 112.1                  |
| Experiment [7] | -                  | -                      | -                      | -                      | -                      | -                      | -                      | -                      |
| Sr$^+$ | $a_0^{(0)}$(5S$_{1/2}$) | $a_0^{(0)}$(5P$_{1/2}$) | $a_0^{(0)}$(5P$_{3/2}$) | $a_0^{(2)}$(5P$_{1/2}$) | $a_0^{(2)}$(5P$_{3/2}$) | $a_0^{(0)}$(4D$_{3/2}$) | $a_0^{(2)}$(4D$_{3/2}$) | $a_0^{(0)}$(4D$_{5/2}$) | $a_0^{(2)}$(4D$_{5/2}$) |
| Main  | 85.73                  | -39.94                  | -28.44                  | 11.33                  | 53.83                  | 34.25                  | 53.63                  | 46.33                  |
| Core  | 4.98                   | 4.98                   | 4.98                   | -                      | 4.98                   | 4.98                   | 4.98                   | 4.98                   |
| Core-valence | $-0.19$               | 0.0                    | 0.0                    | -                      | $-1.77 \times 10^{-2}$ | -                      | $-2.79 \times 10^{-2}$ | -                      |
| Tail  | 1.97 $\times 10^{-2}$ | 3.70                   | 2.67                   | -0.81                  | 4.95                   | 1.00                   | 3.48                   | 1.01                   |
| Total (Present) | 90.54               | -31.27                  | -20.79                  | 10.52                  | 63.74                  | 35.26                  | 62.08                  | 47.35                  |
| Others [8] | 75.28                | -2.774                  | -0.931                  | 10.12                  | 32.99                  | 17.88                  | 32.81                  | 25.16                  |
| Others [9] | 75.1(5)              | -0.75(70)               | 1.02(64)                | 10.31(28)              | 32.0(3)                | -17.43(23)             | 31.8(3)                | -24.51(29)             |
| Experiment [10] | 75.3(4)              | -                      | -                      | -                      | -                      | -                      | -                      | -                      |
| Ba$^+$ | $a_0^{(0)}$(6S$_{1/2}$) | $a_0^{(0)}$(6P$_{1/2}$) | $a_0^{(0)}$(6P$_{3/2}$) | $a_0^{(2)}$(6P$_{1/2}$) | $a_0^{(2)}$(6P$_{3/2}$) | $a_0^{(0)}$(5D$_{3/2}$) | $a_0^{(2)}$(5D$_{3/2}$) | $a_0^{(0)}$(5D$_{5/2}$) | $a_0^{(2)}$(5D$_{5/2}$) |
| Main  | 114.19                 | 6.85                   | 32.00                  | 5.87                   | 39.71                  | 21.92                  | 42.42                  | 30.37                  |
| Core  | 9.35                   | 9.35                   | 9.35                   | -                      | 9.35                   | -                      | 9.35                   | -                      |
| Core-valence | $-0.38$               | 0.0                    | 0.0                    | -                      | $-2.35 \times 10^{-2}$ | -                      | $-3.87 \times 10^{-2}$ | -                      |
| Tail  | 1.66 $\times 10^{-2}$ | 4.26                   | 4.18                   | -1.17                  | 4.76                   | 1.00                   | 4.80                   | 1.47                   |
| Total (Present) | 123.18              | 20.46                  | 45.53                  | 4.70                   | 53.80                  | -22.92                 | 56.53                  | -31.83                 |
| Others [12] | 124.26(1.0)         | -                      | -                      | -                      | 48.81(46)              | -24.62(28)             | 50.67(58)              | -30.85(31)             |
| Experiment [13] | 123.88(5)         | -                      | -                      | -                      | -                      | -                      | -                      | -                      |

Table I lists the contributions from the “Main”, core, valence-core and “Tail” components to the static values of $\alpha_r$ for all the considered alkaline ions. The final values are compared with other available theoretical and experimental values. Transitions up to the $3S-6P$, $3P-6S$, $3P-6d$, $3D-6P$ and $3D-7F$ are included into the "Main" contribution for Mg$^+$ ion.

Institute of standards and technology (NIST) database [8], we determine the "Main" contributions to valence correlations of $\alpha_r$s of the $nS_{1/2}$, $nP_{3/2,1/2}$ and $nD_{3/2,5/2}$ states in the considered alkaline earth metal ions. In Table I we list the contributions from the “Main”, core, valence-core and “Tail” components to the static values of $\alpha_r$ for all the considered alkaline ions. The final values are compared with other available theoretical and experimental values. Transitions up to the $3S-6P$, $3P-6S$, $3P-6d$, $3D-6P$ and $3D-7F$ are included into the "Main" contribution for Mg$^+$ ion. As seen from Table I the ground state dipole polarizability values obtained for the Mg$^+$ ion are very close to the values estimated by Mitroy and Zhang [9]. They evaluate the non-relativistic values of polarizabilities by diagonalizing the semi-empirical Hamiltonian in a large dimension single electron basis. We notice that there is a large difference between our polarizability results for $3D_{3/2}$ and $3D_{5/2}$ states and hence the non-relativistic values calculated by them are unfavorable. Snow [7] deduced the static polarizability for the ground state of the Mg$^+$ ion from the fine structure of high Rydberg levels. Their $\alpha^{(0)}$ value
of 35.02(0.04) \(a_0^3\) agrees well with our result of 35.04 \(a_0^3\). For \(Ca^+\) ion transitions up to the \(4S - 7P\), \(4P - 7S\), \(4P - 6d\), \(3D - 7P\) and \(3D - 7F\) are included into the "Main" contribution. While examining polarizabilities in case of the \(Ca^+\) ion, we notice that our calculation for the ground state polarizability is in the agreement with the result obtained from experimental spectral analysis by Chang [10]. Also, a comparison of our calculated polarizabilities for this ion with the calculations done using combination of many-body perturbation theory and SD scaled method by Safronova et al. [9] shows very good agreement. Moreover, our result for the ground state is in consistent agreement with the results calculated by Tang and co-workers [8]. However, a discrepancy has been observed between our results and other calculations among the \(P\) state polarizabilities this ion. We notice that the polarizabilities of the \(P\) states are very small due to substantial cancellations between some large contributions to the total polarizability. The final values are, thus, very sensitive to these cancellations. Next, we compare our polarizability results for the \(Sr^+\) ion in Table [9]. Transitions up to the \(5S - 8P\), \(5P - 8S\), \(5P - 7d\), \(4D - 8P\) and \(3D - 7F\) are included into the "Main" contribution for this ion. Mitroy and coworkers [11] have used a non-relativistic method using a sum-over-states approach to determine polarizabilities of the \(S\), \(P\) and \(D\) states of \(Sr^+\). It is evident from Table [9] that our ground state dipole polarizability is in agreement with their result. However, it may not be proper to compare their non-relativistic values of the polarizabilities for the \(4D_{5/2}\) and \(4D_{3/2}\) states just by including corrections from the relativistic effects with the non-relativistic values against our fully relativistic calculations. However, the static dipole polarizabilities calculated for the ground and \(4D\) state of the \(Sr^+\) ion using an \(ab\) \textit{initio} relativistic coupled-cluster method [12] are in close agreement with our results. There are no direct experimental values available to compare with these results. The polarizability values for the \(S\), \(P\) and \(D\) states of the \(Sr^+\) ion, derived by combining the experimental results with oscillator strength sums by Barklem and O’Mara [13], has a considerable discrepancy with our present results. In \(Ba^+\) ion, transitions up to the \(6S - 8P\), \(6P - 8S\), \(6P - 6d\), \(5D - 8P\) and \(5D - 7F\) are included into the "Main" contribution. The high-precision ground state polarizability measurement for \(Ba^+\), achieved by using a novel technique, based on the resonant excitation Stark ionization spectroscopy [14], is in very good agreement with our work. To summarize, the above analysis clearly justifies that our calculations of dipole polarizabilities in the considered alkaline earth metal ions are accurate enough to predict the magic wavelengths in these ions reliably.

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