# Parity nonconservation in ytterbium ion

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We consider parity nonconservation (PNC) in singly ionized ytterbium (Yb$^+$) arising from the neutral current weak interaction. We calculate the PNC electric dipole transition amplitude ($E1_{\text{PNC}}$) and the properties associated with it using relativistic coupled-cluster theory. $E1_{\text{PNC}}$ for the $[4f^{14}]\,{}^2 6s \to [4f^{14}]\,{}^2 5d_{3/2}$ transition in Yb$^+$ has been evaluated to within an accuracy of 5%. The improvement of this result is possible. It therefore appears that this ion is a promising candidate for testing the standard model of particle physics.

Parity nonconservation (PNC) has been observed in a number of neutral atoms; the latest being Yb [1,2]. The combined experimental and theoretical results for Cs PNC is the most accurate to date [3]. It is in agreement with the standard model (SM) of particle physics. The experiment on Cs PNC also reports the observation of the nuclear anapole moment (NAM) [3,4]. For more stringent tests of the SM, either the accuracy of the PNC data from Cs must be improved or very-high-precision measurements should be carried out on other candidates. Exploiting the remarkable advances in laser cooling and single-ion-trapping techniques, experiments have been proposed to measure PNC in these systems [5,6]. Both Ba$^+$ [5,6] and Ra$^+$ [7–9] are already under consideration for such experiments. Moreover, the PNC nucleon-nucleon coupling constant related to the NAM obtained from Cs PNC and nuclear data do not agree [4], and this clearly calls for further investigation of these results. In these circumstances, it would certainly be desirable to explore PNC in heavy atomic ions [9]. Apart from Ba$^+$ and Ra$^+$, we had also suggested Pb$^+$ as a possible candidate for PNC measurement [10]. The study of PNC in the $[4f^{14}]\,{}^2 6s \to [4f^{14}]\,{}^2 5d_{3/2}$ transition in Yb$^+$ was suggested by one of us over a decade ago [11] and it is currently being experimentally investigated at Los Alamos National Laboratory [12].

Assuming that the PNC light shift in the above transition in Yb$^+$ can be measured to sub-one-percent accuracy, it would certainly be desirable to determine the accuracy to which $E1_{\text{PNC}}$ can be calculated for this transition. This knowledge is necessary for choosing a system for investigating atomic PNC. In alkali-metal atoms and alkaline-earth-metal ions, the low-lying energy levels which are the singly excited states from the ground state usually make the dominant contributions to the $E1_{\text{PNC}}$ amplitude. Therefore, a typical sum-over-state approach considering only a few important singly excited intermediate states can give a reasonably accurate result. However, Yb$^+$ has a number of doubly excited low-lying intermediate states, and therefore it would not be prudent to use a sum-over-states approach for this ion.

In this Rapid Communication, we employ the relativistic coupled-cluster (RCC) method to calculate $E1_{\text{PNC}}$ using an approach that circumvents summing over intermediate

states [13]. We also present the results of our calculations of the excitation energies and the lifetimes for the $[4f^{14}]\,{}^2 6p_{1/2,3/2}$ state and the electric quadrupole moments of the $[4f^{14}]\,{}^2 6s \to [4f^{14}]\,{}^2 5d_{3/2}$ transition, which is necessary for evaluating the PNC light shift associated with this transition in Yb$^+$. We analyze the role of the electron correlation effects in $E1_{\text{PNC}}$ and compare them with those in Ba$^+$ [13] and Ra$^+$ [7].

In Fig. 1, we present a diagram of the low-lying energy levels of Yb$^+$, mentioning lifetimes of the important states and transitions that can be induced by lasers for the measurement of PNC. As shown in the figure, the lifetimes of the $5d_{3/2,5/2}$ states are fairly large [14–16].

The largest contribution to $E1_{\text{PNC}}$ in the $[4f^{14}]\,{}^2 6s \to [4f^{14}]\,{}^2 5d_{3/2}$ transition comes from the nuclear-spin-independent (NSI) neutral weak current interaction between the electrons and the nucleus due to the exchange of the $Z_0$ boson. The Hamiltonian for this interaction is given by

$$H_{\text{PNC}} = \frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho_{\text{nuc}}(r), \tag{1}$$

where $G_F$ (=2.219 × 10$^{-14}$ in a.u.) is the Fermi constant that quantifies the strength of the weak interaction, $\rho_{\text{nuc}}$ is the nuclear density which is evaluated using the Fermi distribution, $\gamma_5$ is the Dirac matrix, $N$ is the neutron number of the atomic system, and $Q_W$ is known as the weak nuclear charge. As the strength of the weak interaction is very small compared to the electromagnetic interactions in an atomic system; it can be treated as a first-order perturbation. The wave function of an atomic state with a single valence electron $v$ can be expressed as

$$|\Psi_v\rangle = |\Psi_v^{(0)}\rangle + G_F |\Psi_v^{(1)}\rangle, \tag{2}$$

with $G_F$ representing the perturbed parameter and $|\Psi_v^{(0)}\rangle$ and $|\Psi_v^{(1)}\rangle$ being the wave functions corresponding to the the Dirac-Coulomb Hamiltonian ($H_{\text{DC}}$) and its first-order correction due to the PNC weak interaction, respectively. In our RCC approach, we write

$$|\Psi_v\rangle = e^T [1 + S_v] |\Phi_v\rangle, \tag{3}$$

where $|\Phi_v\rangle$ is the Dirac-Fock (DF) wave function obtained by appending the valence electron $v$ to the closed-shell-configuration reference state $|\Phi_0\rangle$ (i.e., $[4f^{14}]$ in the present system) and $T$ and $S_v$ are the core-virtual and valence-virtual excitation operators, respectively. In this work, we have
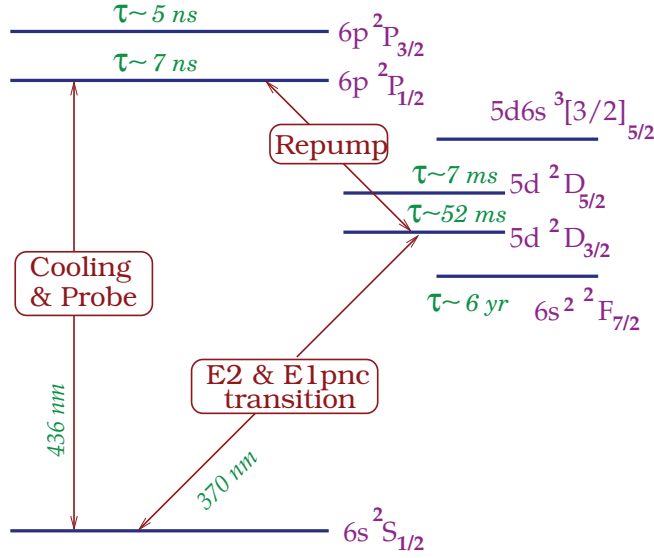
FIG. 1. (Color online) Schematic of energy levels in Yb$^+$ with transitions shown in red lines and that can be induced by different lasers for measurement of the parity nonconservation effect. Lifetimes of different states are denoted by $\tau$.

considered all possible single and double excitations (CCSD method) by taking the operators

$$T = T_1 + T_2 \text{ and } S_v = S_{1v} + S_{2v}, \tag{4}$$

where subscripts 1 and 2 stand for the single and double excitations, respectively. We also consider contributions from triple excitations involving the valence electron by defining the following operator:

$$S_{3v} = \frac{H_{DC}T_2 + H_{DC}S_{2v}}{\varepsilon_p + \varepsilon_q + \varepsilon_r - \varepsilon_v - \varepsilon_a - \varepsilon_b}, \tag{5}$$

where $\varepsilon$ represents the orbital energy and $p,q,r$ and $a,b$ represent the virtual and occupied orbitals, respectively. When $S_{3v}$ is used only to improve the CCSD wave functions, it is referred to as the CCSD(T) method and when its contributions are also estimated in the property evaluation, it is referred to lo-CCSDvT method [17]. Furthermore, we separate the $T$ and $S_v$ operators to represent the unperturbed and perturbed wave functions as

$$T = T^{(0)} + G_F T^{(1)} \text{ and } S_v = S_v^{(0)} + G_F S_v^{(1)}, \tag{6}$$

where the superscripts 0 and 1 denote unperturbed and perturbed operators, respectively. In an explicit form, we can write

$$\left|\Psi_v^{(0)}\right\rangle = e^{T^{(0)}}\left[1 + S_v^{(0)}\right]|\Phi_v\rangle, \tag{7}$$

and $$\left|\Psi_v^{(1)}\right\rangle = e^{T^{(0)}}\left[T^{(1)}\left(1 + S_v^{(0)}\right) + S_v^{(1)}\right]|\Phi_v\rangle. \tag{8}$$

The RCC equations for the correlation energy and the cluster amplitude equations for both the unperturbed and perturbed wave functions have been given in some of our earlier papers (for example, see [13,17]).

An atomic property can be determined in the RCC framework by evaluating the matrix element of an operator $O$ corresponding to that property:

$$\langle O \rangle_{fi} = \frac{\langle \Phi_f | \left[1 + S_f^{(0)\dagger}\right] \mathcal{O}_0 \left[1 + S_i^{(0)}\right] | \Phi_i \rangle}{\sqrt{\mathcal{N}_f \mathcal{N}_i}}, \tag{9}$$

where $\mathcal{O}_0 = e^{T^{(0)\dagger}} O e^{T^{(0)}}$ and $\mathcal{N}_v = \langle \Phi_v | [1 + S_v^{(0)\dagger}] \mathcal{N}_0 [1 + S_v^{(0)}] | \Phi_v \rangle$ with $\mathcal{N}_0 = e^{T^{(0)\dagger}} e^{T^{(0)}}$. Expectation values are determined by taking $f = i$.

The expression for $E1_{PNC}$ between $|\Psi_f\rangle$ and $|\Psi_i\rangle$ after keeping terms up to linear in $G_F$ is given by

$$E1_{PNC} = G_F \frac{\langle \Psi_f^{(0)} | D | \Psi_i^{(1)} \rangle + \langle \Psi_f^{(1)} | D | \Psi_i^{(0)} \rangle}{\sqrt{\langle \Psi_f^{(0)} | \Psi_f^{(0)} \rangle \langle \Psi_i^{(0)} | \Psi_i^{(0)} \rangle}} \tag{10}$$

for the electric dipole (E1) operator $D$, which in the RCC approach leads to

$$\frac{E1_{PNC}}{G_F} = \frac{\langle \Phi_f | \left[1 + S_f^{(0)\dagger}\right] \mathcal{D}_0 \left[T^{(1)}\left(1 + S_i^{(0)}\right) + S_i^{(1)}\right] | \Phi_i \rangle}{\sqrt{\mathcal{N}_f \mathcal{N}_i}}$$
$$+ \frac{\langle \Phi_f | \left[S_f^{(1)\dagger} + \left(1 + S_f^{(0)\dagger}\right) T^{(1)\dagger}\right] \mathcal{D}_0 \left[1 + S_i^{(0)}\right] | \Phi_i \rangle}{\sqrt{\mathcal{N}_f \mathcal{N}_i}}.$$

In Table I, we present results for different properties using our CCSD(T) method. The results for the appropriate properties can be used for estimating the uncertainty of our $E1_{PNC}$ result. We also compare our results with previous calculations and experimental results wherever possible. We analyze the results briefly below.

*Basis functions.* We have considered up to 17 $s$, $p$, $d$, and $f$ and 14 $g$ orbitals using Gaussian-type orbital basis functions. A Fermi-nuclear charge distribution is used to determine the nuclear potential and density.

*Excitation energies.* We have given excitation energies (EEs) in Table I corresponding to the transitions that are important in obtaining an accurate value for the $E1_{PNC}$ result and the lifetimes of excited states. Among them the EE of the $6s_{1/2} \rightarrow 6p_{1/2}$ transition contributes significantly to the $E1_{PNC}$ result, which is obtained to an accuracy of around 4% in this work. All our results are compared with the third order many-body perturbation theory (MBPT(3)) results of Safronova and Safronova [18] and also with experimental values [19].

*E1 matrix elements.* It is important to find the accuracy of the E1 matrix elements that contribute to $E1_{PNC}$. We have presented the important E1 matrix elements in the above table. Our results compare reasonably well with previous calculations [18,26]. In [18], two different approaches were considered to obtain these results, which differ from each other substantially. We have compared our results with Mani and Angom (their published results [26] have been corrected [20]). We combine our E1 matrix elements with the experimental wavelengths to determine the lifetimes of the important intermediate states (i.e., the $6p$ $^2P_{1/2}$ and $6p$ $^2P_{3/2}$ states) and compare them with the measured values in order to test their accuracies. Using our calculated E2 and M1 amplitudes (i.e., 20.70 and 1.15 a.u., respectively) for the $6p_{3/2} \rightarrow 6p_{1/2}$ transition, we find the lifetimes of the $6p$ $^2P_{1/2}$ and $6p$ $^2P_{3/2}$

TABLE I. Comparison of different properties in $^{171}$Yb$^+$ from the present and other works (given up to second decimal place). Uncertainties are given inside the parentheses.

| Transitions | This Work | Others | Experiment |
|---|---|---|---|
| | Excitation energies (in cm$^{-1}$) | | |
| $6s_{1/2} \to 6p_{1/2}$ | 28 109(1000) | 28 048[a] | 27 061.82[b] |
| $6s_{1/2} \to 6p_{3/2}$ | 31 604(800) | 31 411[a] | 30 392.23[b] |
| $6s_{1/2} \to 7p_{1/2}$ | 63 518(200) | 63 227[a] | 63 706.25[b] |
| $6p_{1/2} \to 5d_{3/2}$ | 4879(800) | 6810[a] | 4101.02[b] |
| $6p_{3/2} \to 5d_{3/2}$ | 8375(950) | 10 173[a] | 7431.43[b] |
| $6p_{3/2} \to 5d_{5/2}$ | 7015(1000) | 8962[a] | 6059.54[b] |
| $7p_{3/2} \to 5d_{3/2}$ | 41 502(1500) | 43 175[a] | 42 633.30[b] |
| | E1 Matrix Elements (in a.u.) | | |
| $6s_{1/2} \to 6p_{1/2}$ | 2.72(1) | 2.68 or 2.73,[a] 2.76[c] | |
| $6s_{1/2} \to 6p_{3/2}$ | 3.83(1) | 3.77 or 3.84,[a] 3.87[c] | |
| $6s_{1/2} \to 7p_{3/2}$ | 0.18(2) | 0.15 or 0.04[a] | |
| $6p_{1/2} \to 5d_{3/2}$ | 3.06(2) | 2.97 or 3.78,[a] 3.19[c] | |
| $6p_{3/2} \to 5d_{3/2}$ | 1.35(2) | 1.31 or 1.55,[a] 1.40[c] | |
| $6p_{3/2} \to 5d_{5/2}$ | 4.23(3) | 4.12 or 4.77,[a] 4.39[c] | |
| $7p_{1/2} \to 5d_{3/2}$ | 0.17(2) | 0.08 or 0.12[a] | |
| | E2 Matrix Elements (in a.u.) | | |
| $6s_{1/2} \to 5d_{3/2}$ | 10.2(5) | | |
| $6s_{1/2} \to 5d_{5/2}$ | 12.9(7) | | 12(1) |
| States | $A_{\text{hyf}}$ constants (in MHz) | | |
| $6s_{1/2}$ | 13 332(1000) | 13 172,[a] 12 730[d] | 12 645(2)[d] |
| $6p_{1/2}$ | 2516(400) | 2350,[a] 2317[d] | 2104.9(1.3)[d] |
| $6p_{3/2}$ | 322(20) | 311.5,[a] 391[d] | 877(20)[e] |
| $7p_{1/2}$ | 861(50) | 807.4[a] | |
| $7p_{3/2}$ | 123(15) | 110.8[a] | |
| $5d_{3/2}$ | 447(20) | 400.48[f] | 430(43)[g] |
| $5d_{5/2}$ | −48(15) | −12.58[f] | −63.6(7)[h] |

[a]Reference [18].
[b]Reference [19].
[c]Reference [20].
[d]Reference [21].
[e]Reference [22].
[f]Reference [23].
[g]Reference [24].
[h]Reference [25].

states to be 6.70 and 4.75 ns, which agree reasonably well with the experimental results of 7.1(4) and 5.5(3) ns of Blagoev *et al.* [27], respectively. Also, the branching ratio of the decay rate of the $6p\,^2P_{1/2}$ state to the $5d\,^2D_{3/2}$ state has been reported to be 0.0483 with 9% uncertainty [15] and it agrees well with our result of 0.0439.

*E2 matrix elements.* We have also determined the E2 matrix elements of the $6s_{1/2} \to 5d_{3/2}$ and $6s_{1/2} \to 5d_{5/2}$ transitions which are needed in evaluating the PNC light shift. No other results are available for comparison. Taylor *et al.* have measured the lifetimes of the $5d\,^2D_{5/2}$ state to be 7.2(3) ms with a branching ratio to the $^2F_{7/2}$ state of 0.83(3) [16]. From their measurements, we estimate the E2 matrix element of the $6s_{1/2} \to 5d_{5/2}$ transition to be 12(1) a.u. and our result is in agreement with that. Therefore, we expect that our E2 transition amplitude for the $6s_{1/2} \to 5d_{3/2}$ transition will also be of similar accuracy.

TABLE II. $E1_{\text{PNC}}$ results in Yb$^+$ in $10^{-11}iea_0(-Q_W/N)$ using different approximations.

| Result | Method | | | |
|---|---|---|---|---|
| | DF | CCSD | CCSD(T) | lo-CCSDvT |
| $E1_{\text{PNC}}$ | 6.5311 | 8.5126 | 8.4702 | 8.4704 |

*Hyperfine structure constants.* We have presented the magnetic dipole hyperfine structure constants ($A_{\text{hyf}}$) of the low-lying singly excited states of $^{171}$Yb$^+$. They are also compared with other calculations and experimental results. Our results are comparatively larger than the experimental values, but all the measurements are relatively old. A large disagreement between experimental and all theoretical results of the $6p\,^2P_{3/2}$ state calls for verification of these results using new experimental techniques. However, the accuracies of our results for obtaining a reasonable estimate of $E1_{\text{PNC}}$ are currently acceptable. For high-precision results, it would be necessary to improve the accuracies of the calculations.

$E1_{\text{PNC}}$ *result.* We turn here to our $E1_{\text{PNC}}$ calculation of the $6s_{1/2} \to 5d_{3/2}$ transition where the correlation effects seem to be significant. It can be seen from Table II that the $E1_{\text{PNC}}$ result increases by 30% and 29% at the CCSD and CCSD(T) levels, respectively. So there are some cancellations between the correlation contributions coming via the CCSD and CCSD(T) methods.

We now proceed to discuss the trends of the correlation effects by considering the contributions from different RCC terms. In Table III, we give contributions from the DF and individual CCSD(T) terms. By relating the important CCSD(T) terms to their corresponding lower-order MBPT counterparts, we can identify the correlations effects that are significant. As seen in Table III, three different classes of RCC terms are of crucial importance in arriving at the final result. The $\mathcal{D}_0 T_1^{(1)}$ term represents a subclass of core-valence correlations, whose contribution in the present case is slightly

TABLE III. Contributions (Contr.) to $E1_{\text{PNC}}$ result [in $\times 10^{-11}iea_0(-Q_W/N)$] in Yb$^+$ for the DF and CCSD(T) methods as initial ($i = 6s\,^2S_{1/2}$) and final ($f = 5d\,^2D_{3/2}$) perturbed states. Results given as "Norm" and "Others" refer to contributions from normalization of the wave functions and RCC terms that are not mentioned explicitly, respectively. Subscripts c and vir represent contributions from core and virtual orbitals, respectively.

| Method | Initial State | Contr. | Final State | Contr. |
|---|---|---|---|---|
| DF | $(H_{\text{PNC}}D)_c$ | 0.6441 | $(DH_{\text{PNC}})_c$ | $-3.3 \times 10^{-7}$ |
| | $(DH_{\text{PNC}})_{\text{vir}}$ | 5.8870 | $(H_{\text{PNC}}D)_{\text{vir}}$ | $-4.3 \times 10^{-5}$ |
| RCC | $T_1^{(1)\dagger}\mathcal{D}_0$ | 0.6745 | $\mathcal{D}_0 T_1^{(1)}$ | 0.0070 |
| | $\mathcal{D}_0 S_{1i}^{(1)}$ | 7.1973 | $S_{1f}^{(1)\dagger}\mathcal{D}_0$ | 1.3424 |
| | $\mathcal{D}_0 S_{2i}^{(1)}$ | $-0.2929$ | $S_{2f}^{(1)\dagger}\mathcal{D}_0$ | $-0.2022$ |
| | $S_{1f}^{(0)\dagger}\mathcal{D}_0 S_{1i}^{(1)}$ | 0.5115 | $S_{1f}^{(1)\dagger}\mathcal{D}_0 S_{1i}^{(0)}$ | $-0.0788$ |
| | $S_{2f}^{(0)\dagger}\mathcal{D}_0 S_{1i}^{(1)}$ | $-0.3682$ | $S_{1f}^{(1)\dagger}\mathcal{D}_0 S_{2i}^{(0)}$ | $-0.0617$ |
| | $S_{1f}^{(0)\dagger}\mathcal{D}_0 S_{2i}^{(1)}$ | 0.0004 | $S_{2f}^{(1)\dagger}\mathcal{D}_0 S_{1i}^{(0)}$ | $-0.0165$ |
| | $S_{2f}^{(0)\dagger}\mathcal{D}_0 S_{2i}^{(1)}$ | 0.0271 | $S_{2f}^{(1)\dagger}\mathcal{D}_0 S_{2i}^{(0)}$ | 0.0096 |
| | Others | $-0.6261$ | | 0.7078 |
| | Norm | $-0.2911$ | | $-0.0670$ |

larger than the DF result that is denoted as $(DH_{PNC})_c$. As we have previously discussed [13,17], $\mathcal{D}_0 S_{1v}^{(1)}$ effectively considers contributions from singly excited states with $(DH_{PNC})_{vir}$ as its leading term and involves contributions from important pair-correlation and a class of core-polarization effects. Clearly this contribution through the perturbed $5d\,{}^2D_{3/2}$ state at the DF level is negligible but, after including electron correlation effects, its contribution becomes large. The other important contributions coming via $\mathcal{D}_0 S_{2v}^{(1)}$ are from the core polarization effects involving doubly excited states such as $4f^{13}\,({}^2F_{5/2})\,6s^2$ and $4f^{13}\,({}^2F_{7/2})\,5d6s$. A sizable amount of contribution comes collectively from certain higher order RCC terms given as "Others." Contributions from the normalization of the wave functions (given as "Norm") are also not small.

A detailed comparative study of the trends of the correlation effects in $E1_{PNC}$ amplitudes of the $s_{1/2} \rightarrow 5d_{3/2}$ transitions in Yb$^+$ and similar transitions in Ba$^+$ and Ra$^+$ will be reported elsewhere. However, there is an important point that we would like to highlight here. There is a cancellation between $\mathcal{D}_0 S_{1v}^{(1)}$ and its complex conjugate (c.c.) term in Ba$^+$ and Ra$^+$ but, in contrast in the present case, it adds up. Therefore, the net correlation contribution is larger in Yb$^+$ than other two ions.

Analyzing results from Table III, we find that the leading contributions from $\mathcal{D}_0 T^{(1)} +$ c.c. through the core electrons, $[\mathcal{D}_0 S_{1i}^{(1)} + S_{1f}^{(0)\dagger} \mathcal{D}_0 S_{1i}^{(1)}] +$ c.c. as in the form of the single excitations of the valence electrons and the double-excitation terms $[\mathcal{D}_0 S_{2i}^{(1)} + S_{1f}^{(0)\dagger} \mathcal{D}_0 S_{2i}^{(1)} + S_{2f}^{(0)\dagger} \mathcal{D}_0 S_{2i}^{(1)}] +$ c.c. are around

8%, 101%, and 9% (with opposite sign), respectively. The uncertainties in the contributions from the core and doubly excited states are taken as the differences of the CCSD and lo-CCSD(T) results. Uncertainties from the singly excited states are estimated from the errors of various physical quantities, which are given in Table I, and taking into account their contributions with appropriate weights. With those uncertainties, we estimate the $E1_{PNC}$ amplitude for the $6s\,{}^2S_{1/2} \rightarrow 5d\,{}^2D_{3/2}$ transition in Yb$^+$ to be $8.5(5) \times 10^{-11}\,iG_F ea_0(-Q_W/N)$. The results can be improved by including the triple and quadruple hole-particle excitations in the framework of general-order RCC theory [28].

In conclusion, Yb$^+$ appears to be a promising candidate for the study of atomic PNC. By employing the RCC method in the singles, doubles, and partial triples approximation, we have estimated various atomic properties including the $E1_{PNC}$ amplitude. Our preliminary investigation suggests that it is feasible to obtain theoretical results in this system with high accuracy after suitable modifications to our present method, which has yielded a result that is about 5% accurate. A different trend for correlation effects is found in the present case than for Ba$^+$ and Ra$^+$, which are the two ions that were previously studied using the same method.

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