# Benchmark Calculations of the Energy Spectra and Oscillator Strengths of the Beryllium Atom 

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#### Abstract

In this work, we present a series of benchmark variational calculations for the ground and 19 lowest bound excited singlet $S$ and $P$ states of the beryllium atom. The nonrelativistic wave functions of the states that represent the motion of the nucleus and the four electrons around the center of mass of the atom are expanded in terms of up to 17000 all-particle explicitly correlated Gaussians. The Gaussians are optimized independently for each state. The leading relativistic corrections to the energy levels are computed in the framework of the perturbation theory and they explicitly include the nuclear recoil effects. We also calculate the leading quantum electrodynamics (QED) corrections for each considered state. Using the obtained energy levels and the corresponding wave functions, we compute the transition frequencies, transition dipole moments, and oscillator strengths. A comparison with the available experimental data shows very good agreement. The results of this most comprehensive set of calculations of spectroscopic accuracy for Be to date may open up new applications pertinent to the precision tests of QED, determination of the nuclear charge radius, and modeling matter-radiation equilibria of the beryllium gas that has relevance to the physics of interstellar media.


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Key words: all-electron explicitly correlated Gaussian functions; beryllium atom; oscillator strengths; transition dipole moments; transition frequencies.

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## 1. Introduction

Atomic spectra recorded from astrophysical observations provide rich information on the composition of interstellar objects. Properties such as abundances of elements, their densities, temperature, and other physical parameters can be inferred from these spectra. ${ }^{1,2}$ Based on these properties, models of the chemical and physical transformations can be constructed to explain the phenomena observed in interstellar media. Various space missions that have carried out instruments for very precise measurements of the incoming interstellar radiation have provided a wealth of spectral data for the analysis. However, for the analysis to be carried out with sufficient accuracy, it has to be aided by high-resolution atomic spectra obtained through precision measurements performed in the laboratory and by spectra obtained with high-accuracy theoretical calculations. As more of such new reference data become available, the probing of the physical and chemical conditions of astrophysical objects can be extended to a wider range of interstellar domains.

The present work is concerned with the first-principle quantum-mechanical calculations of the oscillator strengths of atomic inter-state transitions. Accurate values of inter-statetransition oscillator strengths to be used in astrophysical analysis are needed to carry out various astrophysical applications and for
the modeling of interstellar media. Data provided so far have often been insufficiently complete and not accurate enough for the analysis of, for example, stellar atmospheres and plasmas. Continuous progress in the development of new computational methods provides the capability to perform more accurate oscillator strength calculations. However, it takes the combined efforts of theorists and experimentalists to generate data sufficiently accurate for astrophysical applications, as the values obtained from the calculations have to be checked against the laboratory measurements for accuracy and precision. It also happens that the oscillator strengths obtained in current high-precision quantum-mechanical calculations are often considerably more accurate than the measured values, which provides ground for the interplay between the theory and experiment and may lead to re-measurements. Moreover, the present calculations of the oscillator strengths of Be take into account the finite nuclear mass and, thus, can clearly discriminate between various Be isotopes. Previous calculations for lithium, beryllium, and boron atoms (see Refs. 3-6) show that the total uncertainty of the transition energies calculated with explicitly correlated wave functions is smaller than the isotope shifts. Thus, oscillator strengths can be reliably calculated for different isotopes. While, to the best of our knowledge, it is not yet possible to experimentally measure the isotopic shifts of the oscillator strengths for any of the fewelectron atoms or ions, such measurements may become possible in the future.

The accuracy of the calculations of atomic oscillator strengths is primarily dependent on the quality of the wave functions used in the calculations. One needs to go beyond the simplest Hartree-Fock model and account for a large fraction of the electron correlation effects to obtain quality oscillator strengths. Wave functions obtained with various methods have been used to calculate the oscillator strengths. In principle, by including the majority of the electron correlation effects, one should be able to obtain almost exact wave functions in the calculations. However, as obtaining the exact solution of the Schrödinger equation is only possible for one-electron atomic systems, some inaccuracy is always present in the results of the calculations.

Among the methods used to calculate the oscillator strengths for the atomic electronic transitions, the MCHF method has been most frequently used. For example, Fleming et al. ${ }^{7-9}$ implemented the multi-configurational Dirac-Fock/Dirac-Hartree-Fock (MCDF/MCDHF) method in the CIV3 code ${ }^{10}$ and used it in their atomic oscillator-strength calculations. For the beryllium atom, oscillator-strength calculations were performed by Tachiev and Froese Fischer ${ }^{11}$ using the aforementioned method. Their results were confirmed by Ynnerman and Froese Fischer ${ }^{12}$ in their independent MCDF/MCDHF calculations.

The calculations presented in this work focus on the electronic transitions involving ${ }^{1} S$ and ${ }^{1} P$ states of the beryllium atom. The transition energies and the corresponding oscillator strengths are calculated with high accuracy using variationally optimized Gaussian functions that explicitly depend on the distances between the electrons, i.e., the so-called explicitly correlated Gaussian functions (ECGs). The calculations include the leading relativistic and quantum-electrodynamics effects and are performed with an approach where the finite mass of the nucleus is directly incorporated in the Hamiltonian representing the system. This Hamiltonian is used to generate the nonrelativistic wave function and the
corresponding energy for each considered state of the system. The nonrelativistic wave function is expanded in terms of all-particle ECGs, where the term all-particle refers to both electrons and the nucleus.

Different types of explicitly correlated basis functions have been used in the calculations of atomic ground and excited states for several decades now. It has been shown that these types of functions have a clear advantage over single-particle orbitals in calculations aiming to generate almost exact solutions to the Schrödinger equation. For two- and three-electron atomic systems, the best results have been obtained with Hylleraas-type explicitly correlated functions. ${ }^{13}$ For example, for the ground state of helium, the calculations with the Hylleraas basis, in particular, its variant that includes the logarithmic terms that help describe the proper analytic behavior of the wave function at the three-particle coalescence point, yielded the total nonrelativistic ground-state energy with the accuracy exceeding 40 decimal figures. ${ }^{14-19}$ Results obtained with Hylleraas-type basis sets for lithium are accurate up to 15 digits. ${ }^{4,20-22}$

The most accurate results for atoms and ions with four electrons, including beryllium, have been obtained with the all-electron explicitly correlated Gaussian functions. ${ }^{23-27}$ In our recent two works, we used ECGs to calculated some lowest ${ }^{1} S$ and ${ }^{1} P$ states of the beryllium atom. The calculations included the leading relativistic and quantum electrodynamics (QED) corrections. The corrections were calculated using the perturbation theory at the first-order level with the zero-order wave function being the nonrelativistic wave function obtained variationally with the finite-nuclear-mass (FNM) approach mentioned before. With that, the relativistic corrections included contributions from the so-called recoil effects, i.e., the effects due to the dependency of the relativistic corrections on the finite mass of the nucleus. The frequencies of the inter-state transitions calculated for the four lowest ${ }^{1} S$ states considered in Ref. 26 agreed with the experimental values to $0.02-0.09 \mathrm{~cm}^{-1}$. Similar accuracy was achieved in the calculations for the ${ }^{1} P$ states in Ref. 27.

The main task carried out in the present work is the development of the algorithm for calculating the oscillator strengths for atomic $S-P$ transitions. It is applied to calculate the oscillator strengths for the ${ }^{1} S \rightarrow{ }^{1} P$ and ${ }^{1} P \rightarrow{ }^{1} S$ transitions in beryllium. In the first step of the calculations, ECG basis sets for ${ }^{1} S$ and ${ }^{1} P$ states are generated in an iterative process, in which the size of the basis for each state is increased gradually while performing a thorough optimization of both the added basis functions and the functions already included in each basis. The procedure for enlargement of the basis set and variational optimization of the ECG exponential parameters was described previously in Refs. 26 and 27. Due to the use of the analytical energy gradient determined with respect to the parameters of the procedure, the variational energy minimization can be carried out very efficiently. The availability of the analytical gradient in our ECG atomic variational calculations is an important feature that allows us to achieve very high accuracy of the results.

The $2 s^{21} S_{0} \rightarrow 2 s 2 p{ }^{1} P_{1}$ transition has been calculated with rather high accuracy before. Puchalski et al. ${ }^{23}$ used ECG to perform high-precision calculations of the $2 s^{21} S_{0} \rightarrow 2 s 2 p^{1} P_{1}$ transition energy and obtained the value of $42565.441(11) \mathrm{cm}^{-1}$. The calculations included the leading relativistic, QED, and finite-nuclearmass corrections. Their calculated transition energy agrees with the recent saturated absorption measurement of this transition at
42565.4501 (13) $\mathrm{cm}^{-1}$ performed by Cook et al. ${ }^{28}$ The oscillator strength of the transition, however, was not reported by Puchalski et al. On the experimental side, one should mention the precise measurements of the energy levels of the ${ }^{9} \mathrm{Be}$ isotope of beryllium by Bozman et al. ${ }^{29}$ and the measurements of several beryllium transitions performed by Johansson. ${ }^{30}$ The energy for the $2 s^{21} S_{0} \rightarrow 2 s 2 p{ }^{1} P_{1}$ transition obtained in Johansson's experiment was $42565.35(18) \mathrm{cm}^{-1}$. An important conclusion that emerged from comparing the calculated $2 s^{21} S_{0} \rightarrow 2 s 2 p{ }^{1} P_{1}$ transitions energy by Puchalski et al. and the measured values was that the highprecision atomic transition-energy calculations have to account for the QED effects in addition to the relativistic and finite-nuclear-mass (FNM) effects in order to achieve an accuracy approaching that of high-precision experiments. For example, the QED contribution to the $2 s^{21} S_{0} \rightarrow 2 s 2 p{ }^{1} P_{1}$ excitation energy determined by Puchalski et al. was equal to $1.048(9) \mathrm{cm}^{-1}$. The FNM, relativistic, and QED effects are included in the calculations performed in this work.

This work is structured as follows. In Sec. 2, we provide a brief description of the approach used in the calculations. This includes the formulas for the FNM nonrelativistic Hamiltonian used in the calculations, the ECG basis function used for expanding the wave functions of the $S$ and $P$ states considered in this work, and the oscillator strength calculated for the considered interstate $S \rightarrow P$ and $P \rightarrow S$ transitions. Some details concerning the computational implementation of the formulas, as well as the strategy used in the optimization of the ECG non-linear parameters, are also described in Sec. 2. In Sec. 3, the results of the calculations performed in this work are presented. The results concern the ten lowest ${ }^{1} S$ states and the ten lowest ${ }^{1} P$ states of ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$ (i.e., the beryllium atom with an infinitely heavy nucleus). The presented results include the nonrelativistic total energies and relativistic and QED corrections. These quantities are used to calculate the interstate transition energies and the corresponding oscillator strengths. These latter results are compared with the available experimental values. It should be noted that the present results are of benchmark quality, which required several months of continuous computing with hundreds of cores on a parallel computer system. The bulk of the computational time has gone into the optimization of the non-linear parameters of the ECGs, which, as mentioned, are performed variationally with the aid of the analytically calculated energy gradient. The total variational energies for all considered states are notably lower than those obtained in our previous calculations and the calculations performed by others.

In order to put the present calculations in perspective of over 80 years of theoretical works devoted to the calculations of $S$ and $P$ bound states of the beryllium atom, we include Table 1 that shows the progress achieved over the years in calculating the energies of the ground and excited $S$ and $P$ states of the beryllium atom with an infinite-nuclear-mass (INM). Results obtained with different methods are surveyed in the table; most of the methods are based on the variational principle. As one can see, the best results to date have been obtained using ECG expansions of the wave functions. It should be noted that some of the energy values listed in Table 1 have reported uncertainties that are considerably smaller than the actual difference between those values and the corresponding nonrelativistic limit. The reasons for this discrepancy range from overly optimistic assessment of the uncertainty due to the basis truncation to reporting only the statistical errors in the calculations.

TABLE 1. Comparison of nonrelativistic energies of $\infty \mathrm{Be}$ obtained with various theoretical methods: Hartree-Fock (HF), configuration interaction method (CI), poly-detor variational method with exponential functions (PDVM), many-body perturbation theory (MBPT), Hylleraas-type functions (Hy), Hylleraas-Cl method (Hy-Cl), multiconfiguration Hartree-Fock method (MCHF), estimated exact method (EE), explicitly correlated Gaussian functions (ECG), density matrix renormalization group (DMRG), explicitly correlated coupled cluster (CCSDT1-R12), diffusion Monte Carlo (DMC), local Schrödinger equation over free iterative-complement-interaction wave function (LSE-ICI), and explicitly correlated factorizable coupled-cluster method (ECFCC). Some of the quoted values represent an extrapolation to the infinite basis set limit. All energies are in atomic units


TABLE 1. (Continued)

| Work | Year | State | Method | Energy |
| :---: | :---: | :---: | :---: | :---: |
| Sharma et al. ${ }^{64}$ | 2014 | $2{ }^{1} S$ | DMRG | -14.667207 |
| Sims and Hagstrom ${ }^{65}$ | 2014 | $2^{1} S$ | Hy-CI | -14.667356407951 |
|  | 2014 | $2^{1} P$ | ECG | -14.473 451378 |
|  |  | $3{ }^{1} P$ |  | -14.393143528 |
|  |  | $4{ }^{1} P$ |  | -14.361938388 |
| Bubin and Adamowicz ${ }^{66}$ |  | $5{ }^{1} P$ |  | -14.347876275 |
|  |  | $6{ }^{1} P$ |  | -14.340 470145 |
|  |  | $7{ }^{1} P$ |  | -14.336115562 |
|  |  | $8^{1} P$ |  | -14.333 344814 |
| Przybytek and Lesiuk ${ }^{67}$ | 2018 | $2^{1} S$ | ECFCC | -14.667351 |
|  | 2019 | $2^{1} S$ | ECG | -14.667356508(1) |
| Hornyák et al. ${ }^{26}$ |  | $3^{1} S$ |  | -14.418240368(2) |
|  |  | $4{ }^{1} S$ |  | -14.370 087 938(4) |
|  |  | $5{ }^{1} S$ |  | -14.351511736(7) |
|  | 2019 | $2^{1} P$ | ECG | -14.473 4513882 |
|  |  | $3{ }^{1} P$ |  | -14.3931435385 |
|  |  | $4{ }^{1} P$ |  | -14.3619383998 |
|  |  | $5{ }^{1} P$ |  | -14.3478762953 |
| Stanke et al. ${ }^{27}$ |  | $6{ }^{1} P$ |  | -14.340 4701944 |
|  |  | $7{ }^{1} P$ |  | -14.3361157060 |
|  |  | $8^{1} P$ |  | -14.3333453168 |
|  |  | $9^{1} P$ |  | -14.3314759537 |
|  |  | $10^{1} \mathrm{P}$ |  | -14.330 1549127 |
|  |  | $11{ }^{1} P$ |  | -14.329 1852411 |
| Nasiri and Zahedi ${ }^{68}$ | 2020 | $2{ }^{1} S$ | DMC | -14.66734(5) |
|  | 2020 | $3^{1} S$ | Hy-CI | -14.418240346 |
|  |  | $4^{1} S$ |  | -14.370 087890 |
| Sims ${ }^{69}$ |  | $5{ }^{1} S$ |  | -14.351511676 |
|  |  | $6{ }^{1} S$ |  | -14.342 403578 |
|  |  | $7{ }^{1} S$ |  | -14.337266500 |

## 2. Formalism

### 2.1. Nonrelativistic nuclear-mass-dependent Hamiltonian

In this work, we are concerned with the quantum bound states of the atom. These states represent the motion of the particles forming the atom, i.e., the nucleus and the electrons, around the center of mass of the atom. To calculate the wave functions and the corresponding energies of such states, one needs to first derive a Hamiltonian operator that describes the intrinsic motion of all particles in the atom. In our approach, such a Hamiltonian is derived by starting with the standard nonrelativistic laboratory frame Hamiltonian representing the kinetic and potential energies of the nucleus and the electrons and partitioning this Hamiltonian into an operator representing the kinetic energy of the center-of-mass (COM) motion and the remaining part of the Hamiltonian that represents the "internal" state of the system. We call this latter part of the Hamiltonian "the internal Hamiltonian." It is possible to rigorously make this partitioning by a transformation of the coordinates from the laboratory
frame coordinates, which can be, for example, the Cartesian coordinates of the particles forming the atom defined with respect to a particular chosen fixed point in space, to a new set of coordinates. This new set can be chosen to consist, for example, of three coordinates representing the position of the center of mass in the Cartesian laboratory coordinate systems and $3 N-3=3 n$ "internal" coordinates. There are different ways these internal coordinates can be chosen. One possibility is to use the textbook approach employed in solving the Schrödinger equation for the hydrogen atom, where the internal coordinates are the coordinates of the vector with the origin at the proton and the end at the electron. Generalizing this approach to an atom with $n$ electrons, the internal coordinates can be chosen as a superposition of $n$ sets of the coordinates, $\mathbf{r}_{i}, i=1, \ldots, n$, where the $\mathbf{r}_{i}$ is a vector consisting of the $x_{i}, y_{i}$, and $z_{i}$ coordinates with the origin at the nucleus and with the end at electron $i$. Thus, the new coordinate system consists of the lab-frame coordinates of the center of mass, $X_{C M}, Y_{C M}$, and $Z_{C M}$ and the internal coordinates, $\mathbf{r}_{i}, i=1, \ldots, n$.

To separate the full nonrelativistic laboratory frame Hamiltonian into the center-of-mass kinetic-energy operator and the
internal operator, the Hamiltonian is expressed in terms of the new coordinates. This facilitates the separation. The internal Hamiltonian is only a function of the $\mathbf{r}_{i}, i=1, \ldots, n$ coordinates and has the following form (atomic units are assumed throughout):

$$
\begin{equation*}
H_{\mathrm{nr}}^{\mathrm{int}}=-\frac{1}{2}\left(\sum_{i=1}^{n} \frac{1}{\mu_{i}} \nabla_{\mathbf{r}_{i}}^{2}+\sum_{i=1}^{n} \sum_{j \neq i}^{n} \frac{1}{m_{0}} \nabla_{\mathbf{r}_{i}}^{\prime} \nabla_{\mathbf{r}_{j}}\right)+\sum_{i=1}^{n} \frac{q_{0} q_{i}}{r_{i}}+\sum_{i=1}^{n} \sum_{j<i}^{n} \frac{q_{i} q_{j}}{r_{i j}}, \tag{1}
\end{equation*}
$$

where $q_{0}$ is charge of the nucleus, $q_{i}=-1(i=1, \ldots, n)$ are the electron charges, $m_{0}$ is the nuclear mass ( $m_{0}=16424.2055 m_{e}$ for ${ }^{9} \mathrm{Be}$ ), $m_{i}=1$ are the electron masses, $\mu_{i}=m_{0} m_{i} /\left(m_{0}+m_{i}\right)$ is the reduced mass of electron $i, r_{i}$ is the distance between the nucleus and electron $i$, and $r_{i j}=\left|\mathbf{r}_{j}-\mathbf{r}_{i}\right|$ is the distance between electrons $i$ and $j$. In this work, we use the following ${ }^{9} \mathrm{Be}$ nuclear mass: $m_{0}\left({ }^{9} \mathrm{Be}\right)$ $=16424.2055 m_{e},{ }^{70}$ where $m_{e}$ is the mass of the electron. By setting $m_{0}$ to infinity in $H_{\mathrm{nr}}^{\mathrm{int}}$, one gets the INM Hamiltonian that is used in the standard calculations based on the Born-Oppenheimer approximation. Both FNM and INM Hamiltonians are used in the present calculations. When the FNM Hamiltonian is used, both the energy and the wave function depend on the mass of the nucleus. In this work, we report both the finite-mass and infinite-mass results.

Hamiltonian (1) can also be written in a compact matrix form ${ }^{71}$ as

$$
\begin{equation*}
H_{\mathrm{nr}}^{\mathrm{int}}=-\nabla_{\mathbf{r}}^{\prime} \mathbf{M} \nabla_{\mathbf{r}}+\sum_{i=1}^{n} \frac{q_{0} q_{i}}{\mathbf{r}_{i}}+\sum_{i=1}^{n} \sum_{j<i}^{n} \frac{q_{i} q_{j}}{\mathbf{r}_{i j}}, \tag{2}
\end{equation*}
$$

where

$$
\nabla_{\mathbf{r}}=\left(\begin{array}{c}
\nabla_{\mathbf{r}_{1}} \\
\vdots \\
\nabla_{\mathbf{r}_{n}}
\end{array}\right)
$$

is a $n$-component gradient vector and $\mathbf{M}=M \otimes I_{3}$ is the Kronecker product of a $n \times n$ matrix M and $3 \times 3$ identity matrix $I_{3}$. Matrix M has diagonal elements $1 /\left(2 \mu_{1}\right), \ldots$, and $1 /\left(2 \mu_{n}\right)$, while all off-diagonal elements are equal to $1 /\left(2 m_{0}\right)$. The prime symbol denotes the matrix/vector transpose. Hamiltonian (2) is used in the present variational calculations of the nonrelativistic internal energy and the corresponding internal wave function. The internal wave function describing a state of the atom is a function of internal coordinates $\mathbf{r}_{i}, i=1, \ldots, n$.

### 2.2. Basis functions

The basis functions of all-electron explicitly correlated Gaussians are used in the present calculations to construct the spatial parts of the wave functions for the $P$ and $S$ states considered in this work. The $S$-type Gaussians have the following form:

$$
\begin{equation*}
\phi_{k}=\exp \left[-\mathbf{r}^{\prime}\left(A_{k} \otimes I_{3}\right) \mathbf{r}\right] \tag{3}
\end{equation*}
$$

where $A_{k}$ is an $n \times n$ real symmetric matrix, $\otimes$ is the Kronecker product, and $I_{3}$ is a $3 \times 3$ identity matrix. The $P$-type Gaussians have the following form:

$$
\begin{equation*}
\phi_{k}=z_{i_{k}} \exp \left[-\mathbf{r}^{\prime}\left(A_{k} \otimes I_{3}\right) \mathbf{r}\right], \tag{4}
\end{equation*}
$$

where $z_{i_{k}}$ is the $z$-coordinate of the $i$ th electron and $i_{k}$ is the electron label, which varies in the $(1, \ldots, n)$ range and is an adjustable parameter in our calculations. The parameter is specific for each
basis function, $\phi_{k}$, and its value is determined variationally when the ECG basis set is being extended. The above ECG contains an angular pre-exponential factor $z_{i_{k}}$ that makes it suitable for expanding the wave functions of $L=1$ states. The factor is a Cartesian spherical harmonic corresponding to $L=1$ and $M_{L}=0$. A proper $L=1$ ECG is obtained regardless of the value of the electron-label index $i_{k}$ of the pre-exponential $z$ factor. In order to make the initial random choice and subsequent optimization of ECGs more efficient, we treat the index as an additional variational parameter. This is optional, as choosing a fixed value of the electron index of $z$ and not optimizing it, but only optimizing the non-linear exponential ECG parameters, should, in principle, lead to identical results.

The Gaussian basis functions [(3) and (4)] have to be square integrable to represent wave functions of bound $S$ and $P$ states of the atom. This happens when the matrix $A_{k}$ is positive definite. To fulfill this requirement, $A_{k}$ is represented in the Cholesky-factored form ad $A_{k}=L_{k} L_{k}^{\prime}$, where $L_{k}$ is a lower triangular matrix. The $A_{k}$ matrix given in the Cholesky-factored form is always positive definite regardless of the values of the $L_{k}$ matrix elements. Thus, if these matrix elements are used as the variational parameters of the Gaussians and optimized by the minimization of the total energy of the state under the consideration, they can be varied without any constrains from $-\infty$ to $\infty$. This is convenient because any constraint imposed on the variational parameters would make the optimization more cumbersome.

Before either $S$ or $P$ Gaussians given by expressions (3) or (4) are used in expanding the wave function of a state, they have to be appropriately symmetry adapted. In the present approach, we use the spin-free formalism to ensure the correct permutational symmetry properties of each matrix element. For this purpose, an appropriate permutational symmetry projector is constructed and applied to basis functions (3) and (4). To construct the permutationsymmetry projector, the standard procedure involving the Young operators is used. ${ }^{72,73}$ In the case of the singlet $S$ and $P$ states of beryllium, the permutation operator, $Y$, can be chosen in the form $Y=\left(1-P_{13}\right)\left(1-P_{24}\right)\left(1+P_{12}\right)\left(1+P_{34}\right)$, where $P_{i j}$ denotes the permutation of the spatial coordinates of the $i$ th and $j$ th electrons (assuming particle 0 is the nucleus). More details about the generation of the wave function and its variational optimization can be found in Refs. 74 and 75. It should be noted that the variational optimization of the exponential parameters of the $S$ and $P$ basis functions and the electron indices, $i_{k}$, of the $z_{i_{k}}$ factors in the $P$ basis functions is only carried out for the wave functions of the ${ }^{9} \mathrm{Be}$ isotope and then reused in the ${ }^{\infty} \mathrm{Be}$ calculations without reoptimization. Our extensive experience with atomic calculations has shown that just rediagonalizing the Hamiltonian matrix by adjusting the linear variational parameters provides a sufficiently accurate way to account for a relatively small change of the wave function caused by the change in the nuclear mass.

### 2.3. Relativistic and QED corrections

In order to determine atomic transition energies with the accuracy that matches the accuracy of the most precise experiments, the state energies have to be calculated with account for the leading relativistic and quantum-electrodynamics (QED) effects. The most practical way for calculating these effects for few-electron light atoms is to use the standard perturbation theory and to expand the
total energy in powers of the fine-structure constant, $\alpha .{ }^{76,77}$ The first term in this expansion is the nonrelativistic energy of the considered state, $E_{\mathrm{nr}}$,

$$
\begin{equation*}
E_{\mathrm{tot}}=E_{\mathrm{nr}}+\alpha^{2} E_{\mathrm{rel}}^{(2)}+\alpha^{3} E_{\mathrm{QED}}^{(3)}+\alpha^{4} E_{\mathrm{HQED}}^{(4)}+\cdots \tag{5}
\end{equation*}
$$

the second term, $\alpha^{2} E_{\text {rel }}^{(2)}$, represents the leading relativistic corrections, the third term, $\alpha^{3} E_{\mathrm{QED}}^{(3)}$, represents the leading QED corrections, and the fourth term, $\alpha^{4} E_{\mathrm{HQED}}^{(4)}$, represents higher-order QED corrections.

The corrections are evaluated as expectation values of the effective operators representing some physical effects using the nonrelativistic wave function. This wave function can be obtained with either the FNM or INM approach. The $\alpha^{2} E_{\text {rel }}^{(2)}$ term is calculated as the expectation value of the Dirac-Breit Hamiltonian in the Pauli approximation, $H_{\text {rel }}{ }^{78,79}$ In the present calculations of the ${ }^{1} S$ and ${ }^{1} P$ states of beryllium, the Hamiltonian for the relativistic correction, $H_{\text {rel }}$, contains the following terms:

$$
\begin{equation*}
H_{\mathrm{rel}}=H_{\mathrm{MV}}+H_{\mathrm{D}}+H_{\mathrm{OO}}+H_{\mathrm{SS}} \tag{6}
\end{equation*}
$$

where operators $H_{\mathrm{MV}}, H_{\mathrm{D}}, H_{\mathrm{OO}}$, and $H_{\mathrm{SS}}$ represent the massvelocity, Darwin, orbit-orbit, and spin-spin corrections, respectively. As all states considered in this work are singlet states, the spin-orbit interaction vanishes. The explicit form of the operators in the right-hand side of (6) in the internal coordinates, $\mathbf{r}_{i}, i=1, \ldots, n$, is given in our previous publications. ${ }^{26,27}$ It should be mentioned that, when the finite-nuclear-mass approach is used in the calculations of the nonrelativistic energy and the corresponding wave function and of the relativistic corrections, these corrections explicitly depend on the nuclear mass. Thus, the so-called recoil effects are directly accounted for in the calculations.

The leading QED effects in (5) are represented by the $\alpha^{3} E_{\mathrm{QED}}^{(3)}$ term. For an atom, this term accounts for the two-photon exchange, the vacuum polarization, and the electron self-energy effects. The operator has the following form in the internal coordinates:

$$
\begin{align*}
H_{\mathrm{QED}}^{(3)}= & \sum_{\substack{i, j=1 \\
j>i}}^{n}\left[\left(\frac{164}{15}+\frac{14}{3} \ln \alpha\right) \delta\left(\mathbf{r}_{i j}\right)-\frac{7}{6 \pi} \mathscr{P}\left(\frac{1}{r_{i j}^{3}}\right)\right] \\
& +\sum_{i=1}^{n}\left(\frac{19}{30}-2 \ln \alpha-\ln k_{0}\right) \frac{4 q_{0}}{3} \delta\left(\mathbf{r}_{i}\right), \tag{7}
\end{align*}
$$

where the first term represents the so-called Araki-Sucher correction. ${ }^{80-84}$ The correction involves the principal value $\mathscr{P}\left(1 / r_{i j}^{3}\right)$ defined as

$$
\begin{equation*}
\left\langle\mathscr{P}\left(\frac{1}{r_{i j}^{3}}\right)\right\rangle=\lim _{a \rightarrow 0}\left\langle\frac{1}{r_{i j}^{3}} \Theta\left(r_{i j}-a\right)+4 \pi(\gamma+\ln a) \delta\left(\mathbf{r}_{i j}\right)\right\rangle . \tag{8}
\end{equation*}
$$

Here, $\Theta(\cdots)$ is the Heaviside step function and $\gamma=0.577215 \ldots$ is the Euler-Mascheroni constant.

The last term in $H_{\mathrm{QED}}^{(3)}$ represents the electron self-energy. Its dominant contribution is the term involving the so-called Bethe logarithm, $\ln k_{0}$. The main obstacle in computing the QED correction accurately for a multi-electron atomic system comes from $\ln k_{0}$, which is difficult to calculate. However, $\ln k_{0}$ is known to mostly
depend on the contributions from the core electrons. In Sec. 2.4, the procedure used to determine the $\ln k_{0}$ values for the considered states is described.

The last term in expansion (5) is the $E_{\mathrm{HQED}}^{(4)}$ term. It can be calculated as the expectation value of the following approximate operator derived by Pachucki et al. $5^{55,85}$

$$
\begin{equation*}
H_{\mathrm{HQED}}^{(4)}=\pi q_{0}^{2}\left(\frac{427}{96}-2 \ln 2\right) \sum_{i=1}^{n} \delta\left(\mathbf{r}_{i}\right) . \tag{9}
\end{equation*}
$$

$E_{\text {HOED }}^{(4)}$ includes the dominating electron-nucleus one-loop radiative correction but neglects the two-loop radiative, electron-electron radiative, and the higher-order relativistic corrections. The expectation value of (9) only provides a rough approximation to $E_{\mathrm{HQED}}^{(4)}$ for light atoms with the overall error being of the order of $50 \%$.

The expectation values of the $H_{\mathrm{QED}}^{(3)}$ and $H_{\mathrm{HQED}}^{(4)}$ Hamiltonians are calculated in this work with the INM wave functions. This is because the formulas used in the calculations were derived for the clamped nucleus. ${ }^{55,85}$ Thus, the $E_{\mathrm{QED}}^{(3)}$ and $E_{\mathrm{HQED}}^{(4)}$ corrections computed in this work do not include the recoil effects.

Some of the operators used in the calculations of the relativistic and QED effects include singular terms. Examples of such terms are the $\nabla_{\mathbf{r}_{i}}^{4}$ operator in $H_{\mathrm{MV}}$ and the one- and two-electron Dirac delta functions, $\delta\left(\mathbf{r}_{i}\right)$ and $\delta\left(\mathbf{r}_{i j}\right)$, in $H_{\mathrm{D}}, H_{\mathrm{SS}}, H_{\mathrm{QED}}$, and $H_{\mathrm{HQED}}$. The convergence of the expectation values of operators involving singular terms with the number of basis functions used to expand the wave function of the atom is usually much slower than for non-singular operators-the number of converged significant figures is typically about twice smaller. However, there have been studies that proposed neat workarounds to this problem. ${ }^{86-91}$ One way to improve the convergence is to employ expectation value identities, which involve certain global operators whose expectation values coincide with the expectation values of the singular operators in the case of the exact wave function. When an approximate wave function is used instead, the expectation values of those global operators typically converge to the infinite basis set limit at a much faster rate. The original idea was laid out by Drachman ${ }^{91}$ based on the work of Trivedi. ${ }^{90}$ Drachman's approach has been adopted in several works published in recent decades with a good level of success. It has been demonstrated in comparative studies that the convergence of the expectation values of the operators found in the leading relativistic and QED corrections is significantly accelerated by using Drachman's approach. ${ }^{26,92}$ In this work, we also adopt an approach in the same spirit to compute the expectation values of $\delta\left(\mathbf{r}_{i}\right), \delta\left(\mathbf{r}_{i j}\right)$, and $\nabla_{\mathbf{r}_{i}}^{4}$. More details on this can be found in Refs. 5 and 26.

### 2.4. Bethe logarithm fitting

Expression (7) contains a term that includes Bethe logarithm, $\ln k_{0}$. This term represents the dominant part of the electron selfenergy. Accurate calculation of this quantity for multi-electron systems represents a major difficulty. In the case of the beryllium atom, Puchalski et al. ${ }^{4,23}$ studied the three lowest singlet states $\left(2^{1} \mathrm{~S}, 2{ }^{1} \mathrm{P}\right.$, and $3{ }^{1} S$ ) and reported the Bethe logarithms for them. Those are currently the most accurate values available for Be in the literature. For other states, the $\ln k_{0}$ values have been either computed less accurately or not computed at all. Drake and Goldman ${ }^{93}$ showed that the value of the Bethe logarithm for atomic Rydberg states has
the following asymptotic behavior: $A+B / n^{3}$, where $n$ is the principal quantum number and $A$ and $B$ are constants. In this work, we employ a fitting procedure with the above expression to estimate the values of Bethe logarithm for the $S$ and $P$ states using the available $\ln k_{0}$ values for $S\left(2{ }^{1} S, 3{ }^{1} S\right)$ and $P\left(2{ }^{1} P\right)$ states of the Be atom. In our fitting, the Bethe logarithm value for the ground $2^{2} S$ state of $\mathrm{Be}^{+}$ ion $^{94}$ is used as the asymptotic value when $n \rightarrow \infty$. The values of $\ln k_{0}$ we adopted for the $S$ and $P$ states of Be considered in this work are shown in Table 2. To show how those differ from the groundstate value of the hydrogen-like atom, in Table 2, we also list the values of $\ln k_{0} / q_{0}^{2}$ (where $q_{0}$ is the nuclear charge).

### 2.5. Oscillator strength

In the length formalism, the absorption oscillator strength $f_{i f}$ for a transition between an initial state $i$ and a final state $f$ is defined as ${ }^{95,96}$

$$
\begin{equation*}
\left.f_{i f}=\frac{2}{3 g_{i}}\left(\frac{Z_{r}}{Z_{p}}\right) \Delta E_{i f}\left|\left\langle\psi_{i}\right| \boldsymbol{\mu}\right| \psi_{f}\right\rangle\left.\right|^{2}, \tag{10}
\end{equation*}
$$

where $g_{i}=2 J_{i}+1$ is the statistical weight of the lower level, $\Delta E_{i f}$ $=\left|E_{i}-E_{f}\right|$ is the transition energy, $Z_{r}=\frac{q_{0} m_{e}+m_{0}}{n m_{e}+m_{0}}$ and $Z_{p}=\frac{q_{0} m_{e}+m_{0}}{m_{0}}$ are effective radiative charges ( $q_{0}$ is the charge of the nucleus, $m_{0}$ is the nuclear mass, $m_{e}$ is the mass of the electron, and $n$ is the number of electrons), and $\boldsymbol{\mu}$ is the electric dipole-moment operator. For an atom containing $n$ electrons, $\boldsymbol{\mu}=\sum_{i=1}^{n} q_{i} \mathbf{r}_{i}$, where $q_{i}$ and $\mathbf{r}_{i}$ is the charge of electron $i$ and its position in the internal coordinate

TABLE 2. Approximate values of the Bethe logarithm used in the calculations of the QED corrections for the lowest ten ${ }^{1} S$ and ${ }^{1} P$ states of beryllium. All values are in atomic units

| State | Reference | $\ln k_{0}$ | $\ln \left(k_{0} / q_{0}^{2}\right)$ |
| :---: | :---: | :---: | :---: |
| $2{ }^{1} S$ | 4 | 5.75046 | 2.977871 |
| $3{ }^{1} S$ | 4 | 5.75149 | 2.978901 |
| $4^{1} S$ |  | 5.751698 | 2.979109 |
| $5{ }^{1} S$ |  | 5.751783 | 2.979195 |
| $6^{1} S$ |  | 5.751821 | 2.979232 |
| $7{ }^{1} S$ |  | 5.751840 | 2.979252 |
| $8{ }^{1} S$ |  | 5.751851 | 2.979262 |
| $9{ }^{1} S$ |  | 5.751858 | 2.979269 |
| $10^{1} \mathrm{~S}$ |  | 5.751862 | 2.979273 |
| $11{ }^{1} \mathrm{~S}$ |  | 5.751865 | 2.979276 |
| $2{ }^{1} P$ | 4 | 5.752320 | 2.979731 |
| $3{ }^{1} P$ |  | 5.751989 | 2.979401 |
| $4{ }^{1} P$ |  | 5.751909 | 2.979320 |
| $5{ }^{1} P$ |  | 5.751880 | 2.979291 |
| $6{ }^{1} P$ |  | 5.751867 | 2.979279 |
| $7{ }^{1} P$ |  | 5.751861 | 2.979272 |
| $8{ }^{1} P$ |  | 5.751857 | 2.979269 |
| $9{ }^{1} P$ |  | 5.751855 | 2.979266 |
| $10^{1} \mathrm{P}$ |  | 5.751854 | 2.979265 |
| $11^{1} P$ |  | 5.751853 | 2.979264 |
| $2^{2} S \mathrm{Be}^{+}$ | 94 | 5.751849 | 2.979260 |
| $1{ }^{2} \mathrm{SH}$ | 93 | 2.984128 | 2.984128 |

system, respectively. Wave functions $\psi_{i}$ and $\psi_{f}$ are nonrelativistic wave functions obtained in variational calculations using Hamiltonian (2). As the Hamiltonian explicitly depends on the mass of the nucleus, $\psi_{i}$ and $\psi_{f}$ also depend on the nuclear mass, i.e., they are slightly different for ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$. It is worth mentioning that for a charge-neutral system, $\boldsymbol{\mu}$ has the same form in the laboratory Cartesian coordinate system as in the coordinate system where the nucleus is placed at the origin of the internal coordinate system. The transition dipole moment associated with the $i \rightarrow f$ transition can be written in the following form:

$$
\begin{equation*}
\left.\left.\left.\left.\left|\mu_{i f}\right|^{2}=\left|\left\langle\psi_{i}\right| \boldsymbol{\mu}\right| \psi_{f}\right\rangle\left.\right|^{2}=\left|\left\langle\psi_{i}\right| \mu_{x}\right| \psi_{f}\right\rangle\left.\right|^{2}+\left|\left\langle\psi_{i}\right| \mu_{y}\right| \psi_{f}\right\rangle\left.\right|^{2}+\left|\left\langle\psi_{i}\right| \mu_{z}\right| \psi_{f}\right\rangle\left.\right|^{2} . \tag{11}
\end{equation*}
$$

For oscillator strengths, only the transition dipole moments between the $S\left(L=0, M_{L}=0\right)$ and $P\left(L=1, M_{L}=0\right)$ states need to be evaluated [in this case, only the last of the three terms in Eq. (11) is non-zero]. Restricting the calculations to the transitions between the $S\left(L=0, M_{L}=0\right)$ and $P\left(L=1, M_{L}=0\right)$ states only is possible because of symmetry. Effectively, one can obtain the transition dipole moments for all $P$ states with $M_{L}= \pm 1$ by knowing the corresponding values for $M_{L}=0$ (for more information, see Ref. 97).

The transition dipole moment matrix elements with $S$ and $P$ ECG basis functions (3) and (4) can be evaluated in a similar way as the overlap matrix elements (Refs. 74 and 98 contain detailed derivations of the latter, as well as other relevant matrix elements). For the sake of consistency and convenience, below we adopt the same notation scheme as in Refs. 74 and 98. The $z$-component of the transition dipole-moment matrix element between $S\left(L=0, M_{L}=0\right)$ and $P\left(L=1, M_{L}=0\right)$ ECGs can be expressed as

$$
\begin{align*}
\left\langle\hat{P}_{k} \phi_{k}^{(0)}\right| z_{i}\left|\hat{P}_{l} \phi_{l}^{(1)}\right\rangle= & \left\langle\tilde{\phi}_{k}^{(0)}\right| z_{i}\left|\tilde{\phi}_{l}^{(1)}\right\rangle \\
= & \int \exp \left[-\mathbf{r}^{\prime}\left(\tilde{A}_{k} \otimes I_{3}\right) \mathbf{r}\right] z_{i} z_{\tilde{m}_{l}} \\
& \times \exp \left[-\mathbf{r}^{\prime}\left(\tilde{A}_{l} \otimes I_{3}\right) \mathbf{r}\right] d \mathbf{r} \\
= & \int\left(\mathbf{v}^{\prime \prime} \mathbf{r}\right) \exp \left[-\mathbf{r}^{\prime} \tilde{\mathbf{A}}_{k} \mathbf{r}\right]\left(\tilde{\mathbf{v}}^{\prime \prime} \mathbf{r}\right) \exp \left[-\mathbf{r}^{\prime} \tilde{\mathbf{A}}_{l} \mathbf{r}\right] d \mathbf{r} \tag{12}
\end{align*}
$$

Here, $\hat{P}_{k}$ and $\hat{P}_{l}$ are the particle permutation operators for the bra and ket wave functions, respectively, $\mathbf{A}_{k} \equiv A_{k} \otimes I_{3}, \mathbf{A}_{k} \equiv A_{k} \otimes I_{3}$, and $\mathbf{v}^{l} \equiv v^{l} \otimes \boldsymbol{\varepsilon}^{z}$, where $\boldsymbol{\varepsilon}^{z^{\prime}} \equiv(0,0,1) . v^{l}$ is a sparse $n$-component vector with all components equal to zero, except the $m_{l}$ th component. The scalar product of a $3 n$-component vector $\mathbf{v}^{l}$ with another $3 n$ component vector $\mathbf{r}$ yields a single coordinate, $z_{m_{l}}=\mathbf{v}^{l} \mathbf{r}$. The tilde symbol denotes the action of the permutation matrices $\mathbf{P}_{k} \equiv P_{k} \otimes I_{3}$ and $\mathbf{P}_{l} \equiv P_{l} \otimes I_{3}$ corresponding to operators $\hat{P}_{k}$ and $\hat{P}_{l}$ on matrices $\mathbf{A}_{k}, \mathbf{A}_{l}$, and vector $\mathbf{v}^{l}$,

$$
\tilde{\mathbf{A}}_{k}=\mathbf{P}_{k}^{\prime} \mathbf{A}_{k} \mathbf{P}_{k}, \quad \tilde{\mathbf{A}}_{l}=\mathbf{P}_{l}^{\prime} \mathbf{A}_{l} \mathbf{P}_{l}, \quad \tilde{\mathbf{v}}^{l}=\mathbf{P}_{l}^{\prime} \mathbf{v}, \quad z_{\tilde{m}_{k}}=\tilde{\mathbf{v}}^{\prime \prime} \mathbf{r}
$$

The integral in Eq. (12) is given by formula (28) in Ref. 74. In that formula, one needs to make a replacement $v^{k} \rightarrow v^{i}$. With that expression, (12) becomes

$$
\begin{equation*}
\left\langle\tilde{\phi}_{k}^{(0)}\right| z_{i}\left|\tilde{\phi}_{l}^{(1)}\right\rangle=\frac{\pi^{\frac{3 n}{2}}}{2} \frac{v^{i} \tilde{A}_{k l}^{-1} \tilde{v}^{l}}{\left|\tilde{A}_{k l}\right|^{\frac{3}{2}}}, \tag{13}
\end{equation*}
$$

where $\tilde{A}_{k l}=\tilde{A}_{k}+\tilde{A}_{l}$.

### 2.6. Electronic and nuclear densities

The density of particle $i$ in the center-of-mass (COM) coordinate frame is defined as $\rho_{i}(\boldsymbol{\xi})=\left\langle\delta\left(\mathbf{R}_{i}-\mathbf{R}_{\mathrm{cm}}-\boldsymbol{\xi}\right)\right\rangle$, where $i=1, \ldots, N$ and $\mathbf{R}_{\mathrm{cm}}$ is the position vector of the center of mass in the laboratory coordinate frame. In this work, the COM-frame density plots are generated for both the nucleus and the electrons. These density distributions provide a representation of the coupled motion of the nucleus and the electrons around the center of mass in the beryllium atom. If the atom is excited to an increasingly higher Rydberg state, the average radius of the electronic density increases, as manifested by the increasing value of the nucleus-electron average distance and by increasing diffuseness of the COM-frame electron density. At the same time, the electronic density becomes more oscillatory. The oscillations of the electronic density are mirrored by the oscillations of the density of the nucleus in the COM-frame. The matching number of the maxima in the electronic and nuclear densities for a given state occurs because only then the center-ofmass of the atom can remain immobile. However, due to the much larger mass of the nucleus in comparison with the electron mass, the average radius of the nuclear motion around the center of mass is orders of magnitude smaller than the average radius of the electronic motion. A pictorial comparison of the two motions using the electronic and nuclear COM-frame densities is presented Sec. 3. The feature to notice in the plots is the difference in the scales used to plot the electronic and nuclear densities.

## 3. Results

For calculating atomic $S$ and $P$ states in the framework of the ECG method, we used our in-house parallel computer code written in FORTRAN and employing MPI (Message Passing Interface) for communication between parallel processes. The generation of large ECG basis sets together with high accuracy targeted in the calculations requires the use of extended precision (80-bits) arithmetic, which has a hardware implementation in floating-point modules on the $\times 86$ architecture. The calculations performed with extended precision are typically slower by a factor of $2-3$, yet they provide additional 12 bits (or about four decimal figures) of accuracy compared to the standard double precision. Ten singlet $S$ states and ten singlet $P$ states of beryllium have been calculated in this work. In the first step of the calculations, the nonrelativistic wave functions and the corresponding energies are obtained. The calculations are carried out using the standard variational method and involve the generation of sets of basis functions for each state with different sizes. The growing of the basis set for a particular state is performed independently from other states. It involves adding new functions to the set and variationally optimizing their non-linear parameters using a procedure that employs the analytical energy gradient determined with respect to the parameters. More details about the basisset enlargement procedure can be found in our previous works. 99,100 It should be noted that the generation of the basis set for each considered state is by far the most time-consuming step of the calculations. It required about a year of continuous computing using several 100 cores of parallel computer systems equipped with Intel Xeon E5-2695v3 and AMD EPYC 7642 central processing units (CPUs).

In generating the ECG basis sets, the internal Hamiltonian explicitly dependent on the mass of the nucleus of the ${ }^{9} \mathrm{Be}$ isotope, i.e., the FNM Hamiltonian (2) is used. The basis sets are
subsequently used in the calculations for ${ }^{\infty} \mathrm{Be}$. The nonrelativistic energies are shown in Table 3. The results for the ${ }^{9} \mathrm{Be}$ isotope and for ${ }^{\infty} \mathrm{Be}$ are shown as well. For each ${ }^{1} S$ and ${ }^{1} P$ state of ${ }^{9} \mathrm{Be}$, the nonrelativistic energy is reported for three to six basis set sizes to demonstrate the convergence with the number of basis functions. The nonrelativistic energy for ${ }^{\infty} \mathrm{Be}$ is only shown for the largest basis set generated for each state, as the convergence of these values has essentially the same pattern as those for ${ }^{9} \mathrm{Be}$. These energies are compared with the best previously published results. Our largest basis sets range from 16000 basis functions for the lower states to 17000 for the top states. For all states, the values of the nonrelativistic ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$ energies are notably lower than the values previously reported in the literature. For example, for the ground ${ }^{1} S$ state, the present energy value of ${ }^{\infty} \mathrm{Be}$, -14.6673565088 a.u., is lower than the value of -14.667356498 (3) a.u. reported in 2013 by Puchalski et al. ${ }^{23}$ by about $1 \times 10^{-8}$ a.u. For the lowest ${ }^{1} P$ state, the analogous comparison is -14.4734513895 a.u. (our present value) and -14.473451 37(4) a.u. (the value of Puchalski et al. ${ }^{23}$ ). Another example concerns our previous calculations of the five lowest ${ }^{1} S$ states. ${ }^{26}$ The ${ }^{9}$ Be and ${ }^{\infty}$ Be energies obtained in that work with 7000 ECGs for the ground state are -14.666435525 and -14.667356507 a.u., respectively, while the corresponding values obtained in the present calculations are -14.6664355264 and -14.6673565084 a.u., respectively. For $5{ }^{1} S$, the corresponding comparison is -14.3506104259 and -14.3515117339 a.u. (the present calculations) and -14.350610414 and -14.351511722 in the calculations of Hornyák et al. ${ }^{26}$ As one can notice, the improvement is larger for $5^{1} S$ than for the $2{ }^{1} S$ state. In general, due to a larger number of radial nodes in the wave functions of higher excited states, the number of basis functions used in the calculations needs to be increased to maintain a similar level of accuracy for all states. In the present calculations, the number of the basis functions for lower states (up to $n=8$ ) is kept constant and and then increased by 1000 for the higher states $(n=9-11)$. The main factor that limits the increase of the basis size in the present calculations is the CPU time needed to optimize a very large number of ECGs. The results presented in this work reflect a practical limit of the computational resources we have been able to allocate for our calculations at present.

The wave functions calculated for the $S$ and $P$ states for ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$ are used to calculate the expectation values of the operators representing the leading relativistic and QED corrections. The results of the calculations of these quantities are shown in Table 3. The results include the expectation values of the mass-velocity correction, $\left\langle H_{\mathrm{MV}}\right\rangle$, the orbit-orbit correction, $\left\langle H_{\mathrm{OO}}\right\rangle$, and the oneand two-electron $\delta$-functions $\left[\left\langle\delta\left(\mathbf{r}_{i}\right)\right\rangle\right.$ and $\left\langle\delta\left(\mathbf{r}_{i j}\right)\right\rangle$ respectively]. The $\left\langle\mathscr{P}\left(1 / r_{i j}^{3}\right)\right\rangle$ expectation value is also shown. For the ${ }^{9} \mathrm{Be}$ isotope, the results obtained using basis sets with different numbers of ECGs are shown to assess the convergence. For ${ }^{\infty} \mathrm{Be}$, we only show the results obtained with the largest basis sets. The sum of the nonrelativistic energy and the relativistic corrections for each state, $E_{\text {tot }}$, is shown in the last column of Table 3 along with an estimated uncertainty of the result (for more details on uncertainty evaluations, see Ref. 6). $E_{\text {tot }}$ values are used to calculate the interstate transition energies.

The $S \rightarrow P$ and $P \rightarrow S$ transition energies for ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$ calculated using $E_{\text {tot }}$ values taken from Table 3 are shown in Table 4. The values derived from experimental data are also included for
TABLE 3. Convergence of the nonrelativistic energies ( $E_{n r}$ ), expectation values of the mass-velocity correction ( $H_{M V}$ ), $\delta$-functions dependent on interparticle distances, principal value $\left\langle\mathscr{P}\left(1 / r_{i j}^{3}\right)\right\rangle$, and total energies ( $E_{\mathrm{tot}}$ ) with the number of basis functions for the lowest ten ${ }^{1} \mathrm{~S}$ and ${ }^{1} P$ states of beryllium atom $\left({ }^{9} \mathrm{Be}\right.$ and $\left.{ }^{\infty} \mathrm{Be}\right)$. The numbers in parentheses are estimated uncertainties due to the basis truncation error. The tilde sign indicates that expectation value identities were employed to compute the corresponding quantities to improve their convergence. All values are in atomic units

TABLE 3. (Continued)

| State | Isotope | Basis | Reference | $E_{\text {nr }}$ | $\left\langle\tilde{H}_{\mathrm{MV}}\right\rangle$ | 〈 $\mathrm{H}_{\mathrm{OO}}$ 〉 | $\left\langle\tilde{\delta}\left(\mathbf{r}_{i}\right)\right\rangle$ | $\left\langle\tilde{\delta}\left(\mathbf{r}_{i j}\right)\right\rangle$ | $\left\langle\mathscr{P}\left(1 / r_{i j}^{3}\right)\right\rangle$ | $E_{\text {tot }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $4^{1} S$ | ${ }^{9} \mathrm{Be}$ | 14000 |  | -14.369 1855051 | -268.315 505 | -0.932 33762 | 8.776228493 | 0.263512821 | -1.252 93 | -14.371 60487 |
|  |  | 15000 |  | -14.369 1855109 | -268.315 475 | -0.932 33758 | 8.776228516 | 0.263512824 | -1.252 49 | -14.371 160492 |
|  |  | 16000 |  | -14.369 1855129 | -268.315 411 | -0.932 33756 | 8.776228530 | 0.263512826 | -1.25182 | -14.371 160491 |
|  |  | $\infty$ |  | -14.369 1855151 (15) |  |  |  |  |  | -14.371160 493(10) |
|  |  | 7000 | 26 | -14.369 185506 | -268.315 685 | -0.932 33771 | 8.77622847 | 0.263512813 |  |  |
|  |  | $\infty$ | 26 | -14.369 185 514(4) |  |  |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 16000 |  | -14.370 0879367 | -268.381 663 | -0.905 93887 | 8.777846410 | 0.263556605 | -1.252 25 | -14.372062 828 |
|  |  | - |  | -14.3700879397(15) |  |  |  |  |  | -14.372 062 830(10) |
|  |  | 7000 | 26 | -14.370 087930 | -268.381937 | -0.905 93865 | 8.77784635 | 0.263556591 | -1.255 16 |  |
|  |  | $\infty$ | 26 | -14.370087 938(4) |  |  |  |  |  |  |
| $4{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 14600 | 27 | -14.361 0377946 | -267.893 328 | -0.913 54958 | 8.763470236 | 0.262900115 | -1.244 68 | -14.363 007512 |
|  |  | 15500 |  | -14.361 0377961 | -267.893 322 | -0.913 54956 | 8.763470248 | 0.262900116 | -1.244 63 | -14.363 007513 |
|  |  | 16400 |  | -14.3610378022 | -267.893 223 | -0.91354952 | 8.763470279 | 0.262900121 | -1.243 49 | -14.363 007515 |
|  |  | $\infty$ |  | -14.3610378086(36) |  |  |  |  |  | -14.363 007 517(9) |
|  |  | 16400 |  | -14.361 0377999 |  | -0.9135495 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 16400 |  | -14.3619384022 | -267.959 411 | -0.887204 01 | 8.765087272 | 0.262943867 | -1.24392 | -14.363908 028 |
|  |  | - |  | -14.3619384094(36) |  |  |  |  |  | -14.363908 030(9) |
|  |  | 16400 | 27 | -14.361938 3998 |  | -0.887204 0 |  |  |  |  |
| $5{ }^{1} S$ | ${ }^{9} \mathrm{Be}$ | 14000 |  | -14.350 6104118 | -268.272968 | -0.934 16435 | 8.775161626 | 0.263430584 | -1.25427 | -14.352 584783 |
|  |  | 15000 |  | -14.350610 4247 | -268.272 868 | -0.934 16426 | 8.775161679 | 0.263430591 | -1.253 07 | -14.352 584791 |
|  |  | 16000 |  | -14.350610 4259 | -268.272 870 | -0.934 16426 | 8.775161683 | 0.263430592 | -1.253 06 | -14.352 584793 |
|  |  | $\infty$ |  | -14.350610 4274 (8) |  |  |  |  |  | -14.352584 795(11) |
|  |  | 7000 | 26 | -14.350610 414 | -268.273 164 | -0.934 16445 | 8.77516159 | 0.263430571 | -1.255 16 |  |
|  |  | $\infty$ | 26 | -14.350610 428(7) |  |  |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | $\begin{gathered} 16000 \\ \infty \end{gathered}$ |  | $\begin{aligned} & -14.3515117339 \\ & -14.3515117354(8) \end{aligned}$ | $-268.339105$ | -0.907768 57 | 8.776779118 | 0.263474347 | -1.253 49 | $\begin{aligned} & -14.353486014 \\ & -14.353486015(11) \end{aligned}$ |
|  |  | 7000 | 26 | -14.351511722 | -268.339 399 | -0.907768 18 | 8.77677903 | 0.263474325 | -1.25659 |  |
|  |  | $\infty$ | 26 | -14.351511736(7) |  |  |  |  |  |  |
| $5{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 14600 |  | -14.346975 8541 | -268.071 039 | -0.924932 25 | 8.769034122 | 0.263137388 | -1.252 92 | -14.348947726 |
|  |  | 15500 |  | -14.346975 8568 | -268.071 032 | -0.924 93223 | 8.769034146 | 0.263137390 | -1.252 84 | -14.348947 729 |
|  |  | 16400 |  | -14.346975 8672 | -268.070 985 | -0.924932 17 | 8.769034198 | 0.263137397 | -1.252 35 | -14.348947737 |
|  |  | $\infty$ |  | -14.346975 $8784(56)$ |  |  |  |  |  | -14.348947 745(42) |
|  |  | 16400 | 27 | -14.346975 8638 |  | -0.9249322 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 16400 |  | -14.3478762988 | -268.137 180 | -0.898561 42 | 8.770650913 | 0.263181123 | -1.252 78 | -14.349 848081 |
|  |  | $\infty$ |  | -14.3478763100(56) |  |  |  |  |  | -14.349848090(42) |
|  |  | 16400 | 27 | -14.3478762953 |  | -0.898561 4 |  |  |  |  |
| $6{ }^{1} S$ | ${ }^{9} \mathrm{Be}$ | 14000 |  | -14.3415028839 | -268.257 684 | -0.93492953 | 8.774781459 | 0.263400264 | -1.258 15 | -14.343 477035 |
|  |  | 15000 |  | -14.3415029126 | -268.257 307 | -0.934929 21 | 8.774781652 | 0.263400285 | -1.254 90 | -14.343 477046 |
|  |  | 16000 |  | -14.3415029225 | -268.257 223 | -0.934929 13 | 8.774781679 | 0.263400291 | -1.254 12 | -14.343 477052 |
|  |  | $\infty$ |  | -14.3415029331(53) |  |  |  |  |  | -14.343477 060(36) |
|  | ${ }^{\infty} \mathrm{Be}$ | 16000 |  | $-14.3424036766$ | $-268.323452$ | -0.90853440 | 8.776399001 | 0.263444038 | -1.25455 | -14.344377719 |
|  |  | $\infty$ |  | -14.3424036918(53) |  |  |  |  |  | -14.344377 725(36) |

TABLE 3. (Continued)

| State | Isotope | Basis | Reference | $E_{\text {nr }}$ | $\left\langle\tilde{H}_{\mathrm{MV}}\right\rangle$ | $\left\langle H_{\mathrm{OO}}\right.$ 〉 | $\left\langle\tilde{\delta}\left(\mathbf{r}_{i}\right)\right\rangle$ | $\left\langle\tilde{\delta}\left(\mathbf{r}_{i j}\right)\right\rangle$ | $\left\langle\mathscr{P}\left(1 / r_{i j}^{3}\right)\right\rangle$ | $E_{\text {tot }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $6{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 14600 | 2727 | -14.339569 8970 | -268.147264 | -0.92983934 | 8.771437062 | 0.263240458 | -1.25408 | -14.341 542673 |
|  |  | 15500 |  | -14.339569 9048 | -268.147 262 | -0.92983927 | 8.77137104 | 0.263240462 | -1.25405 | -14.341 542680 |
|  |  | 16400 |  | -14.339569 9327 | -268.147 115 | -0.929839 12 | 8.771437280 | 0.263240478 | -1.25223 | -14.341 542702 |
|  |  | $\infty$ |  | -14.339569 964(15) |  |  |  |  |  | -14.34154273(12) |
|  |  | 16400 |  | -14.339569 924 |  | -0.9298393 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 16400 |  | -14.340 4702036 | -268.213 318 | -0.903 45780 | 8.773054048 | 0.263284203 | $-1.25266$ | -14.342 442886 |
|  |  | $\infty$ |  | -14.340 470233 (15) |  |  |  |  |  | -14.342 44291 (12) |
|  |  | 16400 |  | -14.340 470194 |  | -0.903 4578 |  |  |  |  |
| $7{ }^{1} S$ | ${ }^{9} \mathrm{Be}$ | 14000 |  | -14.336365900 9 | -268.251719 | -0.935 32056 | 8.774622594 | 0.263386930 | -1.265 45 | -14.338 339983 |
|  |  | 15000 |  | -14.336366 0542 | -268.251428 | -0.93531972 | 8.774623708 | 0.263387016 | -1.26235 | -14.338 340121 |
|  |  | 16000 |  | -14.3363660919 | -268.251 267 | -0.93531938 | 8.774623968 | 0.263387047 | -1.260 89 | -14.338340 151 |
|  |  | $\infty$ |  | -14.336366132(20) |  |  |  |  |  | -14.338340 18(15) |
|  | ${ }^{\infty} \mathrm{Be}$ | 16000 |  | -14.3372665320 | -268.317496 | -0.90892495 | 8.776241280 | 0.263430793 | -1.26132 | -14.339240504 |
|  |  | $\infty$ |  | -14.337266572(20) |  |  |  |  |  | -14.339 $24054(15)$ |
| $7{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 14600 | 27 | -14.3352154669 | -268.185790 | -0.932 28661 | 8.772641931 | 0.263292332 | -1.25824 | -14.337188708 |
|  |  | 15500 |  | -14.335 2154836 | -268.185794 | -0.93228655 | 8.772642041 | 0.263292336 | -1.25821 | -14.337188725 |
|  |  | 16400 |  | -14.335215 5735 | -268.185 654 | -0.93228611 | 8.772642568 | 0.263292395 | -1.25595 | -14.337188808 |
|  |  | ¢ |  | -14.335215667(50) |  |  |  |  |  | -14.337188 89(42) |
|  |  | 16400 |  | -14.335215 5592 |  | -0.932 2865 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 16400 |  | -14.3361157211 | -268.251 863 | -0.905 89950 | 8.774259420 | 0.263336122 | -1.25638 | -14.338 088869 |
|  |  | $\infty$ |  | -14.336115 820(50) |  |  |  |  |  | -14.33808895(42) |
|  |  | 16400 | 27 | -14.336115706 |  | -0.905 8997 |  |  |  |  |
| $8{ }^{1} S$ | ${ }^{9} \mathrm{Be}$ | 14000 |  | -14.333185 4907 | -268.248 468 | -0.935 55047 | 8.774551560 | 0.263380462 | -1.26685 | -14.335 159515 |
|  |  | 15000 |  | -14.3331857598 | -268.247953 | -0.935 54961 | 8.774553205 | 0.263380607 | -1.262 41 | -14.335 159758 |
|  |  | 16000 |  | -14.3331860056 | -268.247983 | -0.935 54881 | 8.774554820 | 0.263380723 | -1.260 05 | -14.335 160006 |
|  |  | $\infty$ |  | -14.33318626(16) |  |  |  |  |  | -14.335 1603 (15) |
|  | ${ }^{\infty} \mathrm{Be}$ | 16000 |  | -14.3340862510 | -268.314213 | -0.909 15449 | 8.776172170 | 0.263424469 | -1.260 48 | $-14.336060164$ |
|  |  | $\infty$ |  | -14.334086 56(16) |  |  |  |  |  | -14.336060 4(15) |
| $8{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 14600 | 2727 | -14.3324449402 | -268.207584 | -0.93364105 | 8.773310065 | 0.263321187 | -1.26504 | -14.334 418458 |
|  |  | 15500 |  | -14.3324450069 | -268.207593 | -0.93364086 | 8.773310409 | 0.263321197 | -1.26488 | -14.334 418525 |
|  |  | 16400 |  | -14.3324453165 | -268.207487 | -0.93364032 | 8.773312276 | 0.263321319 | -1.26184 | -14.334 418829 |
|  |  | $\infty$ |  | -14.33244563(20) |  |  |  |  |  | -14.334419 1(17) |
|  |  | 16400 |  | -14.332445 2635 |  | -0.933 6411 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 16400 |  | -14.333345 3727 | -268.273702 | -0.907250 64 | 8.774929236 | 0.263365049 | -1.262 28 | -14.335 318798 |
|  |  | $\infty$ |  | -14.33334577(20) |  |  |  |  |  | -14.335319 1(17) |
|  |  | 16400 |  | -14.3333453168 |  | -0.9072510 |  |  |  |  |
| $9{ }^{1} S$ | ${ }^{9} \mathrm{Be}$ | 15000 |  | -14.331080 4172 | -268.245 947 | -0.93570483 | 8.774517184 | 0.263376905 | -1.270 61 | -14.333 054364 |
|  |  | 16000 |  | -14.331080 6115 | -268.246 125 | -0.93570450 | 8.774519513 | 0.263377024 | -1.26988 | -14.333 054565 |
|  |  | 17000 |  | -14.331080 8174 | -268.246315 | -0.93570387 | 8.774521837 | 0.263377150 | -1.26907 | -14.333 054778 |
|  |  | $\infty$ |  | -14.331081 18(18) |  |  |  |  |  | -14.333 0553 (28) |
|  | ${ }^{\infty} \mathrm{Be}$ | 17000 |  | -14.3319809339 | -268.312 545 | -0.909 30887 | 8.776139224 | 0.263420896 | -1.26951 | $-14.333954808$ |
|  |  | $\infty$ |  | -14.331981 33(18) |  |  |  |  |  | $-14.3339551(28)$ |

TABLE 3. (Continued)

| State | Isotope | Basis | Reference | $E_{\text {nr }}$ | $\left\langle\tilde{H}_{\mathrm{MV}}\right\rangle$ | 〈 $H_{\mathrm{OO}}$ 〉 | $\left\langle\tilde{\delta}\left(\mathbf{r}_{i}\right)\right\rangle$ | $\left\langle\tilde{\delta}\left(\mathbf{r}_{i j}\right)\right\rangle$ | $\left\langle\mathscr{P}\left(1 / r_{i j}^{3}\right)\right\rangle$ | $E_{\text {tot }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $9{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 15500 | 2727 | -14.330 5754903 | -268.220 833 | -0.934 45269 | 8.773710101 | 0.263338312 | -1.27153 | -14.332 549183 |
|  |  | 16400 |  | -14.3305759880 | -268.220 546 | -0.934 45125 | 8.773713099 | 0.263338531 | -1.26699 | -14.3325 49665 |
|  |  | 17000 |  | -14.3305761369 | -268.220 503 | -0.93444997 | 8.773713972 | 0.263338625 | -1.265 58 | -14.3325 49811 |
|  |  | $\infty$ |  | -14.330576 29(8) |  |  |  |  |  | -14.3325500(7) |
|  |  | 16400 |  | -14.3305759732 |  | -0.934453 0 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 17000 |  | -14.3314761248 | -268.286721 | -0.908 05838 | 8.775331042 | 0.263382359 | $-1.26601$ | -14.333 449712 |
|  |  | $\infty$ |  | -14.331476 29(8) |  |  |  |  |  | -14.3334499(7) |
|  |  | 16400 |  | -14.3314759537 |  | $-0.9080607$ |  |  |  |  |
| $10^{1} \mathrm{~S}$ | ${ }^{9} \mathrm{Be}$ | 15000 |  | -14.329 6107179 | -268.246720 | -0.935 83794 | 8.774463692 | 0.263372106 | -1.294 41 | -14.331584771 |
|  |  | 16000 |  | -14.329613 2641 | -268.246831 | -0.93582786 | 8.774482339 | 0.263373330 | -1.286 64 | -14.331587302 |
|  |  | 17000 |  | -14.329614 3144 | -268.246463 | -0.935 81878 | 8.774494082 | 0.263374247 | -1.278 20 | -14.331588323 |
|  |  | $\infty$ |  | -14.3296165(11) |  |  |  |  |  | -14.331591(14) |
|  | ${ }^{\infty} \mathrm{Be}$ | 17000 |  | -14.330514 3414 | -268.312 694 | -0.909 42221 | 8.776111519 | 0.263417990 | -1.278 64 | -14.332 488262 |
|  |  | $\infty$ |  | -14.3305166(11) |  |  |  |  |  | -14.332 490(14) |
| $10{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 15500 | 27 | -14.329252 4372 | -268.231374 | -0.93497666 | 8.773943600 | 0.263347709 | -1.295 66 | -14.331226367 |
|  |  | 16400 |  | -14.329255 1006 | -268.230 280 | -0.93496826 | 8.773960301 | 0.263348977 | -1.281 86 | -14.331228959 |
|  |  | 17000 |  | -14.329255 8395 | -268.230 087 | -0.93496709 | 8.773964094 | 0.263349217 | -1.279 28 | -14.331229684 |
|  |  | $\infty$ |  | -14.3292564(3) |  |  |  |  |  | -14.3312305(40) |
|  |  | 16400 |  | -14.329255 0099 |  | -0.9349745 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 17000 |  | -14.330 1557757 | -268.296311 | -0.90857288 | 8.775581319 | 0.263392953 | -1.279 72 | -14.332 129533 |
|  |  | $\infty$ |  | -14.3301563(3) |  |  |  |  |  | -14.332 1303 (40) |
|  |  | 16400 |  | -14.330 1549127 |  | -0.9085776 |  |  |  |  |
| $11{ }^{1} \mathrm{~S}$ | ${ }^{9} \mathrm{Be}$ | 15000 |  | -14.3285360402 | -268.250 503 | -0.935 92220 | 8.774378167 | 0.263364456 | -1.334 33 | -14.330510 390 |
|  |  | 16000 |  | -14.328547 3290 | -268.251558 | -0.93594051 | 8.774457465 | 0.263368146 | -1.321 39 | -14.330521634 |
|  |  | 17000 |  | -14.3285497685 | -268.250 488 | -0.935 93094 | 8.774469172 | 0.263369954 | -1.31173 | -14.330524007 |
|  |  | $\infty$ |  | -14.3285565(34) |  |  |  |  |  | -14.3305304(32) |
|  | ${ }^{\infty} \mathrm{Be}$ | 17000 |  | -14.3294497307 | $-268.316720$ | -0.909 53006 | 8.776086711 | 0.263413679 | $-1.31217$ | -14.331423881 |
|  |  | $\infty$ |  | -14.329 4565 (34) |  |  |  |  |  | -14.3314302(32) |
| $11{ }^{1} P$ | ${ }^{9} \mathrm{Be}$ | 15000 | 27 | -14.3282747305 | -268.236832 | -0.935 34441 | 8.774047267 | 0.263348909 | -1.320 58 | -14.330248804 |
|  |  | 16000 |  | -14.3282766080 | -268.236811 | -0.93534126 | 8.774054107 | 0.263349863 | -1.31840 | -14.330250 672 |
|  |  | 17000 |  | -14.328287870 0 | -268.236605 | -0.935 32084 | 8.774118432 | 0.263354974 | -1.295 65 | -14.330 261848 |
|  |  | $\infty$ |  | -14.328 2909(15) |  |  |  |  |  | -14.3302659(20) |
|  |  | 16400 |  | -14.328285 4223 |  | -0.935 3442 |  |  |  |  |
|  | ${ }^{\infty} \mathrm{Be}$ | 17000 |  | -14.3291877659 | -268.302834 | -0.908922 79 | 8.775735832 | 0.263398707 | -1.296 08 | -14.331 161656 |
|  |  | $\infty$ |  | -14.329 190 8(15) |  |  |  |  |  | -14.3311647(20) |
|  |  | 16400 | 27 | -14.329 1852411 |  | -0.9089403 |  |  |  |  |

TABLE 4. Transition energies, $\Delta E_{i f}\left(\right.$ in $\left.\mathrm{cm}^{-1}\right)$. The numbers in the parentheses are estimated uncertainties due to the basis set truncation and due to neglecting higher order corrections (both uncertainties are considered independent in our estimates). The experimental values, $\Delta E_{\text {if }}^{\mathrm{Exp}}$, have been taken from NIST Atomic Spectra Database (ver. 5.8). ${ }^{101}$ It should be noted that the experimental energy levels for $n^{1} P(n=7-11)$ states in NIST ASD were determined by extrapolation of values with lower $n$ using a quantum-defect expansion formula along the Rydberg series

| Transition | $\Delta E_{i f}\left({ }^{( } \mathrm{Be}\right)$ | $\Delta E_{i f}\left({ }^{9} \mathrm{Be}\right)$ | $\Delta E_{i f}^{\operatorname{Exp}}$ |
| :---: | :---: | :---: | :---: |
| $2{ }^{1} S \rightarrow 2{ }^{1} P$ | 42568.372 (9) | 42 565.443(9) | $42565.4502(10)$ |
| Ref. 4 |  | 42565.441 (11) |  |
| $2{ }^{1} S \rightarrow 3{ }^{1} P$ | $60191.905(7)$ | $60187.444(7)$ | 60 187.443(21) |
| $2{ }^{1} S \rightarrow 4{ }^{1} P$ | 67 039.288(6) | 67 034.814(6) | 67 034.80(3) |
| $2{ }^{1} S \rightarrow 5{ }^{1} P$ | $70125.089(6)$ | 70 120.578(6) | 70120.59 (3) |
| $2{ }^{1} S \rightarrow 6{ }^{1} P$ | $71750.342(6)$ | 71745.796 (6) | 71746.17 (6) |
| $2^{1} S \rightarrow 7^{1} P$ | 72705.938 (11) | 72701.365 (11) | 72 701.8(5) |
| $2{ }^{1} S \rightarrow 8{ }^{1} P$ | 73 313.90(3) | 73 309.31(3) | 73 309.7(5) |
| $2{ }^{1} S \rightarrow 9{ }^{1} P$ | 73 724.12(2) | 73719.51 (2) | 73 709.4(5) |
| $2{ }^{1} S \rightarrow 10{ }^{1} P$ | 74 013.86(8) | 74009.24 (8) | $74009.2(5)$ |
| $2{ }^{1} S \rightarrow 11{ }^{1} P$ | 74 226.3(2) | 74 221.7(2) | 74 221.1(5) |
| $2{ }^{1} P \rightarrow 3{ }^{1} S$ | $12112.435(4)$ | $12111.906(4)$ | $12111.898(21)$ |
| $2{ }^{1} P \rightarrow 4{ }^{1} S$ | 22 681.144(4) | 22 680.000(4) | 22 679.986(21) |
| $2{ }^{1} P \rightarrow 5{ }^{1} S$ | 26 758.283(4) | $26756.894(4)$ | 26 756.84(7) |
| $2{ }^{1} P \rightarrow 6{ }^{1} S$ | 28 757.323(4) | $28755.812(4)$ | 28755.79 (8) |
| $2{ }^{1} P \rightarrow 7{ }^{1} S$ | 29884.811 (5) | $29883.232(5)$ | 29882.92 (18) |
| $2{ }^{1} P \rightarrow 8{ }^{1} S$ | 30582.82 (3) | 30 581.19(3) | 30581.21 (19) |
| $2{ }^{1} P \rightarrow 9^{1} S$ | 31 044.89(2) | 31043.24 (2) | 31 043.1(3) |
| $2{ }^{1} P \rightarrow 10{ }^{1} S$ | 31366.767 | 31365.09 (11) | 31365.0 (3) |
| $2{ }^{1} P \rightarrow 11{ }^{1} S$ | 31 600.4(3) | 31 598.7(3) | 31598.0 (3) |
| $3{ }^{1} S \rightarrow 3{ }^{1} P$ | 5511.098 (3) | 5 510.095(3) | 5 510.094(30) |
| $3{ }^{1} S \rightarrow 4{ }^{1} P$ | 12358.480 (1) | $12357.465(1)$ | 12357.45 (4) |
| $3{ }^{1} S \rightarrow 5^{1} P$ | $15444.282(2)$ | 15 443.230(2) | 15 443.24(4) |
| $3{ }^{1} S \rightarrow 6{ }^{1} P$ | 17 069.534(3) | 17 068.447(3) | 17 068.82(6) |
| $3{ }^{1} S \rightarrow 7{ }^{1} P$ | 18 025.131(10) | 18 024.016(10) | 18 024.4(5) |
| $3{ }^{1} S \rightarrow 8{ }^{1} P$ | 18 633.09(3) | 18 631.96(3) | 18 632.3(5) |
| $3{ }^{1} S \rightarrow 9^{1} P$ | 19 043.31(2) | 19 042.16(2) | 19 032.0(5) |
| $3{ }^{1} S \rightarrow 10{ }^{1} \mathrm{P}$ | 19 333.05(8) | 19331.89 (8) | $19331.8(5)$ |
| $3{ }^{1} S \rightarrow 11{ }^{1} P$ | 19 545.5(2) | 19 544.3(2) | 19 543.7(5) |
| $3{ }^{1} P \rightarrow 4{ }^{1} S$ | $5057.611(2)$ | 5 057.998(2) | 5057.993 (30) |
| $3{ }^{1} P \rightarrow 5{ }^{1} S$ | 9134.750 (2) | 9134.893 (2) | $9134.856(73)$ |
| $3{ }^{1} P \rightarrow 6{ }^{1} S$ | 11 133.790(2) | $11133.811(2)$ | 11133.80 (8) |
| $3{ }^{1} P \rightarrow 7{ }^{1} S$ | 12 261.278(4) | 12 261.230(4) | 12 260.93(18) |
| $3{ }^{1} P \rightarrow 8{ }^{1} S$ | 12 959.28(3) | 12 959.19(3) | 12 959.2(2) |
| $3{ }^{1} P \rightarrow 9^{1} S$ | 13 421.35(2) | 13 421.24(2) | 13 421.1(3) |
| $3{ }^{1} P \rightarrow 10{ }^{1} S$ | 13 743.22(11) | 13743.09 (11) | 13 743.0(3) |
| $3{ }^{1} P \rightarrow 11{ }^{1} S$ | 13 976.8(3) | 13 976.7(3) | 13 976.0(3) |
| $4{ }^{1} S \rightarrow 4{ }^{1} P$ | 1789.7716 (10) | $1789.3714(10)$ | 1789.36 (37) |
| $4{ }^{1} S \rightarrow 5{ }^{1} P$ | 4875.573 (1) | $4875.136(1)$ | 4875.15 (37) |
| $4{ }^{1} S \rightarrow 6{ }^{1} P$ | 6500.826 (2) | $6500.353(2)$ | 6 500.73(64) |
| $4^{1} S \rightarrow 7^{1} P$ | 7 456.422(9) | 7 455.923(9) | 7 456.3(5) |
| $4^{1} S \rightarrow 8{ }^{1} P$ | 8064.38 (3) | 8063.86 (3) | $8064.2(5)$ |
| $4{ }^{1} S \rightarrow 9^{1} P$ | 8474.60 (2) | 8474.06 (2) | 8463.9 (5) |
| $4{ }^{1} S \rightarrow 10{ }^{1} P$ | 8764.35 (8) | 8763.80 (8) | 8763.7 (5) |
| $4{ }^{1} S \rightarrow 11{ }^{1} P$ | 8 976.8(2) | 8 976.2(2) | $8975.6(5)$ |

TABLE 4. (Continued)

| Transition | $\Delta E_{i f}\left({ }^{( } \mathrm{Be}\right)$ | $\Delta E_{i f}\left({ }^{9} \mathrm{Be}\right)$ | $\Delta E_{i f}^{\mathrm{Exp}}$ |
| :---: | :---: | :---: | :---: |
| $4{ }^{1} P \rightarrow 5{ }^{1} S$ | 2 287.3679(9) | 2287.5231 (9) | 2287.50 (76) |
| $4{ }^{1} P \rightarrow 6{ }^{1} S$ | 4 286.4074(10) | 4286.4411 (10) | 4286.45 (85) |
| $4{ }^{1} P \rightarrow 7{ }^{1} S$ | 5413.896 (3) | 5 413.861(3) | 5 413.58(18) |
| $4{ }^{1} P \rightarrow 8{ }^{1} S$ | 6111.90 (3) | $6111.82(3)$ | 6111.87 (19) |
| $4{ }^{1} P \rightarrow 9^{1} S$ | 6 573.97(2) | 6573.87 (2) | 6573.8 (3) |
| $4^{1} \mathrm{P} \rightarrow 10^{1} S$ | 6895.84 (11) | 6895.72 (11) | 6895.7 (3) |
| $4^{1} \mathrm{P} \rightarrow 11^{1} \mathrm{~S}$ | 7129.4 (3) | 7129.3 (3) | 7128.7 (3) |
| $5{ }^{1} S \rightarrow 5{ }^{1} P$ | 798.4338(9) | 798.2415(9) | 798.29(76) |
| $5{ }^{1} S \rightarrow 6{ }^{1} P$ | 2 423.686(2) | 2 423.459(2) | 2 423.87(92) |
| $5{ }^{1} S \rightarrow 7{ }^{1} P$ | 3 379.283(9) | 3 379.028(9) | 3 379.5(5) |
| $5{ }^{1} S \rightarrow 8{ }^{1} P$ | 3987.24 (3) | 3 986.97(3) | 3 987.4(5) |
| $5{ }^{1} S \rightarrow 9{ }^{1} P$ | 4397.46 (2) | 4 397.17(2) | 4387.1 (5) |
| $5{ }^{1} S \rightarrow 10{ }^{1} P$ | 4687.21 (8) | 4686.90 (8) | 4686.9 (5) |
| $5^{1} S \rightarrow 11^{1} P$ | 4899.630 (2) | 4899.3 (2) | $4898.8(5)$ |
| $5{ }^{1} P \rightarrow 6{ }^{1} S$ | $1200.6057(5)$ | $1200.6764(5)$ | 1200.66 (76) |
| $5{ }^{1} P \rightarrow 7{ }^{1} S$ | 2328.094 (2) | 2328.096 (2) | 2327.79 (18) |
| $5{ }^{1} P \rightarrow 8{ }^{1} S$ | 3026.10 (3) | 3 026.06(3) | 3 026.0(2) |
| $5{ }^{1} P \rightarrow 9{ }^{1} S$ | 3488.17 (2) | 3 488.10(2) | 3 488.01(3) |
| $5^{1} \mathrm{P} \rightarrow 10{ }^{1} \mathrm{~S}$ | 3 810.04(11) | 3809.95 (11) | 3809.91 (3) |
| $5{ }^{1} P \rightarrow 11{ }^{1} S$ | 4043.6 (3) | 4043.5 (3) | 4 042.91(3) |
| $6{ }^{1} S \rightarrow 6{ }^{1} P$ | 424.647(2) | 424.541(2) | 424.92(10) |
| $6{ }^{1} S \rightarrow 7^{1} P$ | 1380.243 (9) | 1380.110 (9) | $1380.5(5)$ |
| $6{ }^{1} S \rightarrow 8{ }^{1} P$ | 1988.20 (3) | $1988.05(3)$ | 1988.4(5) |
| $6^{1} S \rightarrow 9^{1} P$ | 2398.42 (2) | 2398.25 (2) | 2388.1 (5) |
| $6{ }^{1} S \rightarrow 10{ }^{1} P$ | 2 688.17(8) | 2 687.99(8) | 2 687.9(5) |
| $6^{1} S \rightarrow 11^{1} P$ | 2900.6 (2) | 2900.4 (2) | $2899.8(5)$ |
| $6^{1} P \rightarrow 7{ }^{1} S$ | 702.8414(10) | 702.8786(10) | 702.21(19) |
| $6{ }^{1} P \rightarrow 8{ }^{1} S$ | $1400.85(2)$ | $1400.84(2)$ | 1400.5 (20) |
| $6{ }^{1} P \rightarrow 9{ }^{1} S$ | 1862.92 (2) | $1862.88(2)$ | $1862.4(3)$ |
| $6^{1} \mathrm{P} \rightarrow 10{ }^{1} \mathrm{~S}$ | 2 184.79(11) | 2184.73 (11) | 2184.3 (3) |
| $6{ }^{1} \mathrm{P} \rightarrow 11^{1} \mathrm{~S}$ | 2 418.4(3) | 2 418.3(3) | 2 417.3(3) |
| $7{ }^{1} S \rightarrow 7^{1} P$ | 252.755(6) | 252.691(6) | 253.4(5) |
| $7{ }^{1} S \rightarrow 8{ }^{1} P$ | 860.72(3) | 860.63(3) | 861.3(5) |
| $7{ }^{1} S \rightarrow 9^{1} P$ | 1270.93 (2) | 1270.83 (2) | $1261.0(5)$ |
| $7{ }^{1} S \rightarrow 10{ }^{1} P$ | 1560.68 (8) | 1560.57 (8) | $1560.8(5)$ |
| $7{ }^{1} S \rightarrow 11^{1} P$ | $1773.1(2)$ | 1773.0 (2) | 1772.7 (5) |
| $7{ }^{1} P \rightarrow 8{ }^{1} S$ | 445.25(2) | 445.27(2) | 444.87(5) |
| $7{ }^{1} P \rightarrow 9^{1} S$ | 907.32(2) | 907.31(2) | 906.8(6) |
| $7{ }^{1} \mathrm{P} \rightarrow 10^{1} \mathrm{~S}$ | 1229.19 (11) | 1229.16 (11) | 1228.7 (6) |
| $7{ }^{1} P \rightarrow 11^{1} S$ | 1462.8 (3) | $1462.8(3)$ | $1461.7(6)$ |
| $8{ }^{1} S \rightarrow 8{ }^{1} P$ | 162.711(6) | 162.669(6) | 163.0(5) |
| $8{ }^{1} S \rightarrow 9^{1} P$ | 572.93(2) | 572.87(2) | 562.7(5) |
| $8{ }^{1} S \rightarrow 10{ }^{1} P$ | 862.67(8) | 862.61(8) | 862.5(5) |
| $8{ }^{1} S \rightarrow 11^{1} P$ | 1075.1(2) | 1075.0 (2) | $1074.4(5)$ |
| $8{ }^{1} P \rightarrow 9^{1} S$ | 299.36(2) | 299.37(2) | 298.9(6) |
| $8{ }^{1} \mathrm{P} \rightarrow 10{ }^{1} \mathrm{~S}$ | 621.23(11) | 621.22(11) | 620.8(6) |
| $8{ }^{1} P \rightarrow 11{ }^{1} S$ | 854.8(3) | 854.8(3) | 853.8(6) |

TABLE 4. (Continued)

| Transition | $\Delta E_{i f}\left({ }^{\infty} \mathrm{Be}\right)$ | $\Delta E_{i f}\left({ }^{9} \mathrm{Be}\right)$ | $\Delta E_{i f}^{\operatorname{Exp}}$ |
| :--- | :---: | :---: | ---: |
| $9^{1} S \rightarrow 9{ }^{1} P$ | $110.856(7)$ | $110.827(7)$ | $100.8(6)$ |
| $9{ }^{1} S \rightarrow 10^{1} P$ | $400.60(6)$ | $400.56(6)$ | $400.6(6)$ |
| $9{ }^{1} S \rightarrow 11^{1} P$ | $613.0(2)$ | $211.02(10)$ | $612.5(6)$ |
| $9^{1} P \rightarrow 10^{1} S$ | $211.01(10)$ | $445.13(2)$ | $221.1(6)$ |
| $9{ }^{1} P \rightarrow 11^{1} S$ | $444.62(2)$ | $78.71(3)$ | $454.1(6)$ |
| $10^{1} S \rightarrow 10^{1} P$ | $78.73(3)$ | $291.1(2)$ | $78.7(6)$ |
| $10^{1} S \rightarrow 11^{1} P$ | $291.2(2)$ | $154.9(2)$ | $290.6(6)$ |
| $10^{1} P \rightarrow 11^{1} S$ | $154.9(2)$ | $57.5(2)$ | $154.3(6)$ |
| $11^{1} S \rightarrow 11^{1} P$ | $57.6(2)$ | $57.6(6)$ |  |

TABLE 5. The squares of the transition dipole moments, $\left|\mu_{i f}\right|^{2}$, and oscillator strengths, $f_{i f}$, between ${ }^{1} S$ and ${ }^{1} P$ states. For $\left|\mu_{i f}\right|^{2}$, the numbers in parentheses are estimated uncertainties due to the basis truncation. The oscillator strength uncertainties are taken as root mean squares of the uncertainties of $\left|\mu_{i f}\right|^{2}$ and $\Delta E_{i f}$. Numbers in square brackets, [ s ], denote a multiplication factor $10^{s}$

| Transition | $\left\|\mu_{i f}\right\|^{2}\left({ }^{\infty} \mathrm{Be}\right)$ | $\left\|\mu_{i f}\right\|^{2}\left({ }^{9} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{9} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{( } \mathrm{Be}\right)^{\mathrm{a}}$ | $f_{i f}\left({ }^{( } \mathrm{Be}\right)^{\mathrm{b}}$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)^{\text {c }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $2{ }^{1} S \rightarrow 2{ }^{1} P$ | $1.063146385(10)[+1]$ | $1.063255365(10)[+1]$ | 1.374689 2(3) [0] | 1.374400 8(3) [0] | 1.375 [0] | 1.38 [0] | 1.380 [0] |
| $2{ }^{1} S \rightarrow 3{ }^{1} P$ | $4.70328(2)[-2]$ | $4.69534(2)[-2]$ | 8.59931(4) [-3] | $8.58206(4)[-3]$ | $9.01[-3]$ | $8.98[-3]$ | 8.985 [-3] |
| $2{ }^{1} S \rightarrow 4{ }^{1} P$ | $1.31961(4)[-3]$ | $1.32966(4)[-3]$ | 2.687 20(9) [-4] | $2.70682(9)[-4]$ | $2.30[-4]$ | $1.20[-4]$ |  |
| $2{ }^{1} S \rightarrow 5{ }^{1} P$ | $4.02652(7)[-3]$ | 4.038 60(7) [-3] | $8.57684(14)[-4]$ | 8.599 94(14) [-4] | 8.10 [-4] | $6.90[-4]$ |  |
| $2{ }^{1} S \rightarrow 6{ }^{1} P$ | $3.62230(13)[-3]$ | $3.63070(13)[-3]$ | $7.8947(3)[-4]$ | $7.9105(3)[-4]$ | 7.50 [-4] | $6.80[-4]$ |  |
| $2{ }^{1} S \rightarrow 7{ }^{1} P$ | $2.76062(14)[-3]$ | $2.76631(14)[-3]$ | $6.0968(3)[-4]$ | $6.1075(3)[-4]$ | $5.90[-4]$ | $5.40[-4]$ |  |
| $2{ }^{1} S \rightarrow 9{ }^{1} P$ | $1.52452(2)[-3]$ | $1.52754(2)[-3]$ | $3.41403(4)[-4]$ | 3.41974(4) [-4] | 3.20 [-4] | 3.07 [-4] |  |
| $2{ }^{1} S \rightarrow 10{ }^{1} P$ | $1.154(2)[-3]$ | $1.156(2)[-3]$ | $2.594(5)[-4]$ | $2.599(5)[-4]$ |  |  |  |
| $2{ }^{1} S \rightarrow 11{ }^{1} \mathrm{P}$ | 8.90(7) [-4] | 8.92(7) [-4] | 2.01(2) [-4] | 2.01(2) [-4] |  |  |  |
| $2{ }^{1} P \rightarrow 3{ }^{1} S$ | $9.6135787(15)$ [0] | $9.6131861(15)$ [0] | $1.1790161(5)[-1]$ | $1.1786293(5)[-1]$ | $1.18[-1]$ | $1.15[-1]$ | 1.147 [-1] |
| $2{ }^{1} P \rightarrow 4{ }^{1} S$ | $4.28048(6)[-1]$ | $4.28054(6)[-1]$ | $9.83015(14)[-3]$ | 9.827 42(14) [-3] | $9.82[-3]$ | $9.80[-3]$ |  |
| $2{ }^{1} P \rightarrow 5{ }^{1} S$ | $1.3407(2)[-1]$ | $1.3408(2)[-1]$ | $3.6324(6)[-3]$ | $3.6317(6)[-3]$ | $3.62[-3]$ | $3.55[-3]$ |  |
| $2{ }^{1} P \rightarrow 6{ }^{1} S$ | $6.7763(2)[-2]$ | 6.777 9(2) [-2] | $1.9731(5)[-3]$ | $1.9729(5)[-3]$ | $1.96[-3]$ | 1.88 [-3] |  |
| $2{ }^{1} P \rightarrow 7{ }^{1} S$ | 4.223 04(9) [-2] | 4.224 96(9) [-2] | 1.277 85(3) [-3] | $1.27805(3)$ [-3] | $1.23[-3]$ | 1.18 [-3] |  |
| $2{ }^{1} P \rightarrow 8{ }^{1} S$ | 2.943 73(5) [-2] | 2.945 90(5) [-2] | $9.11545(15)[-4]$ | $9.11948(15)[-4]$ | $9.08[-4]$ | $8.11[-4]$ |  |
| $2{ }^{1} P \rightarrow 9{ }^{1} S$ | $2.19374(2)$ [-2] | $2.19604(2)$ [-2] | $6.89571(8)[-4]$ | $6.90087(8)[-4]$ | $6.94[-4]$ | $5.92[-4]$ |  |
| $2{ }^{1} \mathrm{P} \rightarrow 10{ }^{1} \mathrm{~S}$ | 1.706(2) [-2] | $1.709(2)[-2]$ | 5.420(7) [-4] | $5.425(7)[-4]$ | 5.62 [-4] |  |  |
| $2{ }^{1} P \rightarrow 11^{1} S$ | 1.370(7) [-2] | $1.372(7)[-2]$ | $4.38(2)[-4]$ | $4.39(2)[-4]$ |  |  |  |
| $3{ }^{1} S \rightarrow 3{ }^{1} P$ | $5.7133428(3)[+1]$ | $5.7139111(3)[+1]$ | 9.564 292(5) [-1] | $9.561174(5)[-1]$ | $9.58[-1]$ | $9.57[-1]$ | $9.465[-1]$ |
| $3{ }^{1} S \rightarrow 4{ }^{1} P$ | $2.76251(5)[-1]$ | $2.76926(5)[-1]$ | $1.03704(2)$ [-2] | 1.039 23(2) [-2] | $9.82[-2]$ | $9.80[-2]$ |  |
| $3{ }^{1} S \rightarrow 5{ }^{1} P$ | 3.153 21(2) [-1] | $3.15718(2)[-1]$ | 1.479 26(8) [-2] | 1.480 66(8) [-2] | 1.45 [-2] | 1.45 [-2] |  |
| $3{ }^{1} S \rightarrow 6{ }^{1} P$ | $2.10353(5)[-1]$ | $2.10571(5)[-1]$ | 1.090 67(2) [-2] | $1.09147(2)[-2]$ | 1.07 [-2] | $1.08[-2]$ |  |
| $3{ }^{1} S \rightarrow 7{ }^{1} P$ | 1.389 96(2) [-1] | $1.39127(2)[-1]$ | $7.61034(14)[-3]$ | 7.615 22(14) [-3] | $7.51[-3]$ | $7.50[-3]$ |  |
| $3{ }^{1} S \rightarrow 8{ }^{1} P$ | $9.5036(5)[-2]$ | $9.5126(5)[-2]$ | $5.3790(3)[-3]$ | $5.3824(3)[-3]$ | $5.29[-3]$ | $4.73[-3]$ |  |
| $3{ }^{1} S \rightarrow 9{ }^{1} P$ | $6.7381(14)[-2]$ | $6.7449(14)[-2]$ | $3.8977(8)[-3]$ | $3.9004(8)[-3]$ | $3.79[-3]$ | $3.87[-3]$ |  |
| $3{ }^{1} S \rightarrow 10{ }^{1} P$ | 4.934(10) [-2] | 4.940(10) [-2] | $2.897(6)[-3]$ | $2.900(6)[-3]$ |  |  |  |
| $3{ }^{1} S \rightarrow 11{ }^{1} \mathrm{P}$ | 3.72(3) [-2] | $3.72(3)[-2]$ | $2.21(2)[-3]$ | $2.21(2)[-3]$ |  |  |  |
| $3{ }^{1} P \rightarrow 4{ }^{1} S$ | $4.060230(3)[+1]$ | 4.059 474(3) [+1] | $2.079214(2)[-1]$ | $2.078480(2)[-1]$ | 2.09 [-1] | $2.12[-1]$ |  |
| $3{ }^{1} P \rightarrow 5{ }^{1} S$ | $2.630541(4)$ [0] | $2.630732(4)[0]$ | $2.433016(3)[-2]$ | $2.432638(3)[-2]$ | 2.43 [-2] | 2.44 [-2] |  |
| $3{ }^{1} P \rightarrow 6{ }^{1} S$ | $7.6127(7)[-1]$ | $7.6140(7)[-1]$ | $8.5820(7)[-3]$ | $8.5813(7)[-3]$ | 8.57 [-3] | $8.59[-3]$ |  |
| $3{ }^{1} P \rightarrow 7{ }^{1} S$ | $3.4078(5)[-1]$ | $3.4087(5)[-1]$ | $4.2308(6)[-3]$ | $4.2308(6)[-3]$ | 4.23 [-3] | $4.22[-3]$ |  |

TABLE 5. (Continued)

| Transition | $\left\|\mu_{i f}\right\|^{2}\left({ }^{\infty} \mathrm{Be}\right)$ | $\left\|\mu_{i f}\right\|^{2}\left({ }^{9} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{9} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)^{\mathrm{a}}$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)^{\mathrm{b}}$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)^{\text {c }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $3{ }^{1} P \rightarrow 8{ }^{1} S$ | $1.8743(3)[-1]$ | $1.8750(3)[-1]$ | $2.4593(4)[-3]$ | 2.459 6(4) [-3] | 2.47 [-3] | $2.44[-3]$ |  |
| $3{ }^{1} P \rightarrow 9{ }^{1} S$ | $1.16185(10)[-1]$ | $1.16245(10)[-1]$ | $1.57889(13)[-3]$ | $1.57930(13)[-3]$ | $1.60[-3]$ | $1.56[-3]$ |  |
| $3{ }^{1} \mathrm{P} \rightarrow 10^{1} \mathrm{~S}$ | 7.791(9) [-2] | 7.796(9) [-2] | 1.084(13) [-3] | $1.085(13)[-3]$ | $1.14[-3]$ |  |  |
| $3{ }^{1} \mathrm{P} \rightarrow 11^{1} \mathrm{~S}$ | 5.53(2) [-2] | $5.54(2)[-2]$ | 7.83(3) [-4] | 7.83(3) [-4] |  |  |  |
| $4^{1} S \rightarrow 4{ }^{1} P$ | $2.6312970(6)[+2]$ | $2.6317086(6)[+2]$ | 1.430513 2(9) [0] | 1.430068 9(9) [0] | 1.43 [0] |  |  |
| $4{ }^{1} S \rightarrow 5{ }^{1} P$ | $1.23043(14)[-1]$ | $1.23764(14)[-1]$ | 1.822 24(20) [-3] | $1.83231(20)[-3]$ | 1.59 [-3] | $1.67[-3]$ |  |
| $4{ }^{1} S \rightarrow 6{ }^{1} P$ | $2.6167(2)[-1]$ | $2.6222(2)[-1]$ | $5.1671(4)[-3]$ | $5.1764(4)[-3]$ | $4.95[-3]$ | $5.10[-3]$ |  |
| $4{ }^{1} S \rightarrow 7{ }^{1} P$ | $1.8571(8)[-1]$ | $1.8600(8)[-1]$ | 4.206(2) [-3] | $4.212(2)[-3]$ | $4.08[-3]$ | $4.17[-3]$ |  |
| $4{ }^{1} S \rightarrow 8{ }^{1} P$ | $1.2563(2)[-1]$ | $1.2580(2)[-1]$ | $3.0774(5)[-3]$ | $3.0808(5)[-3]$ | $2.98[-3]$ | $2.71[-3]$ |  |
| $4{ }^{1} S \rightarrow 9{ }^{1} P$ | 8.726(2) [-2] | 8.738(2) [-2] | $2.246(5)[-3]$ | $2.249(5)[-3]$ | $2.16[-3]$ | $2.23[-3]$ |  |
| $4{ }^{1} S \rightarrow 10{ }^{1} P$ | 6.269(6) [-2] | 6.278(6) [-2] | $1.669(2)[-3]$ | 1.671(2) [-3] |  |  |  |
| $4{ }^{1} S \rightarrow 11{ }^{1} \mathrm{P}$ | 4.65(3) [-2] | 4.66 (3) [-2] | 1.27(9) [-3] | 1.27(9) [-3] |  |  |  |
| $4{ }^{1} P \rightarrow 5{ }^{1} S$ | $1.266409(2)[+2]$ | $1.266156(2)$ [+2] | $2.933007(4)[-1]$ | 2.931 905(4) [-1] | $2.95[-1]$ |  |  |
| $4{ }^{1} P \rightarrow 6{ }^{1} S$ | $8.28777(7)$ [0] | 8.288 28(7) [0] | 3.596 95(3) [-2] | $3.59632(3)[-2]$ | $3.60[-3]$ | $3.61[-3]$ |  |
| $4{ }^{1} P \rightarrow 7{ }^{1} S$ | $2.3120(5)[0]$ | $2.3124(5)[0]$ | $1.2674(3)[-2]$ | $1.2672(3)[-2]$ | 1.27 [-2] | 1.27 [-2] |  |
| $4{ }^{1} P \rightarrow 8{ }^{1} S$ | $1.0092(2)$ [0] | $1.0095(2)$ [0] | $6.2453(11)[-3]$ | $6.2454(11)[-3]$ | $6.27[-3]$ | $6.25[-3]$ |  |
| $4{ }^{1} P \rightarrow 9^{1} S$ | $5.4594(6)[-1]$ | $5.4617(6)[-1]$ | $3.6340(4)[-3]$ | $3.6345(4)[-3]$ | $3.69[-3]$ | $3.63[-3]$ |  |
| $4^{1} \mathrm{P} \rightarrow 10^{1} \mathrm{~S}$ | $3.348(3)[-1]$ | $3.351(3)[-1]$ | $2.338(2)[-3]$ | $2.339(2)[-3]$ | $2.45[-3]$ |  |  |
| $4{ }^{1} \mathrm{P} \rightarrow 11^{1} \mathrm{~S}$ | 2.232(8) [-1] | $2.234(8)[-1]$ | $1.611(6)[-3]$ | 1.612(6) [-3] |  |  |  |
| $5{ }^{1} S \rightarrow 5{ }^{1} P$ | $7.481658(8)[+2]$ | 7.482 926(8) [+2] | 1.814 518(3) [0] | 1.813 946(3) [0] | 1.82 [0] |  |  |
| $5{ }^{1} S \rightarrow 6{ }^{1} P$ | 8.401(5) [-2] | 8.496(5) [-2] | 6.185(3) [-4] | $6.253(3)[-4]$ | 4.78 [-4] |  |  |
| $5{ }^{1} S \rightarrow 7{ }^{1} P$ | $3.272(4)[-1]$ | $3.281(4)[-1]$ | 3.359(4) [-3] | 3.367(4) [-3] | $3.16[-3]$ | $3.32[-3]$ |  |
| $5{ }^{1} S \rightarrow 8{ }^{1} P$ | $2.4207(9)[-1]$ | $2.4248(9)[-1]$ | $2.9318(11)[-3]$ | $2.9359(11)[-3]$ | $2.79[-3]$ | $2.59[-3]$ |  |
| $5{ }^{1} S \rightarrow 9{ }^{1} P$ | $1.673(3)[-1]$ | $1.676(3)[-1]$ | $2.235(4)[-3]$ | $2.237(4)[-3]$ | 2.10 [-3] | $2.22[-3]$ |  |
| $5{ }^{1} S \rightarrow 10{ }^{1} P$ | 1.179(2) [-1] | 1.181(2) [-1] | $1.679(3)[-3]$ | 1.681(3) [-3] |  |  |  |
| $5{ }^{1} S \rightarrow 11{ }^{1} \mathrm{P}$ | 8.57(5) [-2] | 8.59(5) [-2] | 1.28(7) [-3] | 1.28(7) [-3] |  |  |  |
| $5{ }^{1} P \rightarrow 6{ }^{1} S$ | $3.15764(2)[+2]$ | $3.15704(2)[+2]$ | 3.838 54(3) [-1] | $3.83710(3)[-1]$ | $3.86[-1]$ |  |  |
| $5{ }^{1} P \rightarrow 7{ }^{1} S$ | $2.0313(2)[+1]$ | $2.0315(2)[+1]$ | $4.7884(6)[-2]$ | 4.787 6(6) [-2] | 4.79 [-2] |  |  |
| $5{ }^{1} P \rightarrow 8{ }^{1} S$ | 5.4986 (8) [0] | 5.4998 (8) [0] | $1.6848(3)$ [-2] | $1.6847(3)$ [-2] | 1.69 [-2] |  |  |
| $5{ }^{1} P \rightarrow 9{ }^{1} S$ | 2.350(2) [0] | 2.351(2) [0] | 8.299(9) [-3] | 8.300(9) [-3] | $8.45[-2]$ | 8.32 [-3] |  |
| $5{ }^{1} \mathrm{P} \rightarrow 10^{1} \mathrm{~S}$ | 1.257(3) [0] | 1.257(3) [0] | 4.848(12) [-3] | 4.849(12) [-3] | $5.10[-2]$ |  |  |
| $5{ }^{1} \mathrm{P} \rightarrow 11^{1} \mathrm{~S}$ | 7.66(3) [-1] | 7.67(3) [-1] | $3.14(13)[-3]$ | $3.14(13)[-3]$ |  |  |  |
| $6{ }^{1} S \rightarrow 6{ }^{1} P$ | $1.691681(10)[+3]$ | $1.691971(10)[+3]$ | 2.182 081(16) [0] | $2.181379(16)$ [0] | 2.19 [0] |  |  |
| $6{ }^{1} S \rightarrow 7{ }^{1} P$ | 4.85(2) [-2] | 4.96 (2) [-2] | 2.03(9) [-4] | 2.08(9) [-4] | $1.12[-4]$ |  |  |
| $6{ }^{1} S \rightarrow 8{ }^{1} P$ | 4.238(8) [-1] | 4.251(8) [-1] | $2.560(5)[-3]$ | 2.567(5) [-3] | $2.30[-3]$ |  |  |
| $6{ }^{1} S \rightarrow 9{ }^{1} P$ | 3.257(13) [-1] | $3.261(13)[-1]$ | $2.373(9)[-3]$ | $2.375(9)[-3]$ | $2.12[-3]$ |  |  |
| $6{ }^{1} S \rightarrow 10{ }^{1} P$ | 2.272(6) [-1] | $2.276(6)[-1]$ | 1.855(5) [-3] | 1.858(5) [-3] |  |  |  |
| $6{ }^{1} S \rightarrow 11{ }^{1} P$ | $1.606(4)[-1]$ | $1.608(4)[-1]$ | $1.415(3)[-3]$ | 1.417(3) [-3] |  |  |  |
| $6{ }^{1} P \rightarrow 7{ }^{1} S$ | $6.7069(4)[+2]$ | $6.7058(4)[+2]$ | 4.772 9(3) [-1] | $4.7712(3)[-1]$ | 4.79 [-1] |  |  |
| $6{ }^{1} P \rightarrow 8{ }^{1} S$ | $4.231(2)[+1]$ | $4.231(2)[+1]$ | 6.001(2) [-2] | $6.000(2)[-2]$ | $6.03[-2]$ |  |  |
| $6{ }^{1} P \rightarrow 9{ }^{1} S$ | $1.1194(14)[+1]$ | $1.1197(14)[+1]$ | $2.1114(26)[-2]$ | $2.1114(26)[-2]$ | 2.15 [-2] |  |  |
| $6{ }^{1} \mathrm{P} \rightarrow 10{ }^{1} \mathrm{~S}$ | 4.705(3) [0] | 4.708(3) [0] | $1.041(7)[-2]$ | $1.041(7)[-2]$ | 1.10 [-2] |  |  |
| $6{ }^{1} \mathrm{P} \rightarrow 11^{1} \mathrm{~S}$ | 2.485(6) [0] | 2.487(6) [0] | 6.084(16) [-3] | 6.088(16) [-3] |  |  |  |
| $7{ }^{1} S \rightarrow 7{ }^{1} P$ | $3.3165(2)[+3]$ | $3.3170(2)[+3]$ | $2.5462(2)$ [0] | $2.5454(2)$ [0] | 2.56 [0] |  |  |
| $7{ }^{1} S \rightarrow 8{ }^{1} P$ | $1.307(7)[-2]$ | $1.387(7)[-2]$ | 3.418(19) [-5] | 3.624(19) [-5] | $5.00[-8]$ | $5.00[-8]$ |  |
| $7{ }^{1} S \rightarrow 9{ }^{1} P$ | 5.380(8) [-1] | $5.384(8)[-1]$ | $2.077(3)[-3]$ | $2.078(3)[-3]$ | 1.64 [-3] |  |  |

TABLE 5. (Continued)

| Transition | $\left\|\mu_{i f}\right\|^{2}\left({ }^{\infty} \mathrm{Be}\right)$ | $\left\|\mu_{i j}\right\|^{2}\left({ }^{9} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{9} \mathrm{Be}\right)$ | $f_{i f}\left({ }^{( } \mathrm{Be}\right)^{\text {a }}$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)^{\mathrm{b}}$ | $f_{i f}\left({ }^{\infty} \mathrm{Be}\right)^{\mathrm{c}}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $7{ }^{1} S \rightarrow 10{ }^{1} P$ | 4.31(3) [-1] | 4.30(3) [-1] | 2.04(1) [-3] | 2.04(1) [-3] |  |  |  |
| $7{ }^{1} S \rightarrow 11{ }^{1} P$ | 3.00(6) [-1] | 3.00(6) [-1] | 1.62 (3) [-3] | 1.62(3) [-3] |  |  |  |
| $7{ }^{1} P \rightarrow 8{ }^{1} S$ | $1.2699(3)[+3]$ | $1.2697(3)[+3]$ | 5.725 2(13) [-1] | $5.7232(13)[-1]$ | 5.75 [-1] |  |  |
| $7{ }^{1} P \rightarrow 9^{1} S$ | 7.869(7) [+1] | 7.869(7) [+1] | 7.229(6) [-2] | 7.228(6) [-2] | 7.33 [-2] |  |  |
| $7{ }^{1} P \rightarrow 10{ }^{1} S$ | 2.045(5) [+1] | $2.046(5)[+1]$ | 2.546 (6) [-2] | 2.546 (6) [-2] | 2.68 [-2] |  |  |
| $7{ }^{1} P \rightarrow 11^{1} S$ | 8.46(4) [0] | 8.47(4) [0] | 1.25(5) [-2] | 1.25(5) [-2] |  |  |  |
| $8^{1} S \rightarrow 8{ }^{1} P$ | 5.888 2(12) [+3] | 5.888 9(12) [+3] | $2.9102(6)$ [0] | 2.909 1(6) [0] | 2.94 [0] |  |  |
| $8{ }^{1} S \rightarrow 9{ }^{1} P$ | 1.6(4) [-3] | 1.3(4) [-3] | 2.8(8) [-6] | 2.3(8) [-6] | 1.47 [-6] |  |  |
| $8{ }^{1} S \rightarrow 10{ }^{1} P$ | 6.59(4) [-1] | 6.57(4) [-1] | $1.73(1)[-3]$ | $1.72(1)[-3]$ |  |  |  |
| $8{ }^{1} S \rightarrow 11{ }^{1} P$ | 5.42(14) [-1] | 5.41(14) [-1] | 1.77(5) [-3] | 1.76(5) [-3] |  |  |  |
| $8^{1} P \rightarrow 9^{1} S$ | $2.2070(8)[+3]$ | $2.2065(8)[+3]$ | $6.6895(24)[-1]$ | $6.6869(24)[-1]$ | 6.73 [-2] |  |  |
| $8{ }^{1} P \rightarrow 10^{1} S$ | 1.349(7) [+2] | 1.349(7) [+2] | 8.49(4) [-2] | 8.48(4) [-2] | 8.82 [-2] |  |  |
| $8{ }^{1} P \rightarrow 11^{1} \mathrm{~S}$ | $3.47(5)[+1]$ | 3.47 (5) [+1] | 3.00(5) [-2] | 3.00(5) [-2] |  |  |  |
| $9^{1} S \rightarrow 9{ }^{1} P$ | $9.7199(11)[+3]$ | $9.7207(11)[+3]$ | 3.273 0(4) [0] | 3.271 6(4) [0] | 3.34 [0] |  |  |
| $9^{1} S \rightarrow 10{ }^{1} P$ | 5.(5) [-2] | 5.(5) [-2] | 6.(6) $[-5]$ | 6.(6) $[-5]$ |  |  |  |
| $9{ }^{1} S \rightarrow 11^{1} P$ | 8.(2) [-1] | 8.(2) [-1] | 1.(3) $[-3]$ | 1.(3) $[-3]$ |  |  |  |
| $9{ }^{1} P \rightarrow 10{ }^{1} S$ | 3.583(13) [+3] | 3.582(13) [+3] | 7.656(27) [-1] | 7.652(27) [-1] | 7.80 [-1] |  |  |
| $9{ }^{1} P \rightarrow 11^{1} S$ | $2.19(6)[+2]$ | 2.19(6) [+2] | $9.84(26)[-2]$ | $9.85(26)[-2]$ |  |  |  |
| $10^{1} S \rightarrow 10{ }^{1} P$ | 1.519(5) [+4] | 1.519(5) [+4] | 3.632(12) [0] | 3.630(12) [0] |  |  |  |
| $10^{1} S \rightarrow 11^{1} P$ | 1.(2) [-1] | 1.(2) [-1] | 1.(2) [-4] | 1.(2) [-4] |  |  |  |
| $10{ }^{1} \mathrm{P} \rightarrow 11{ }^{1} \mathrm{~S}$ | 5.50(7) [+3] | 5.49(7) [+3] | 8.62(11) [-1] | 8.61(11) [-1] |  |  |  |
| $11^{1} S \rightarrow 11^{1} P$ | 2.28(4) [+4] | 2.28(4) [+4] | 3.98(7) [0] | 3.98(7) [0] |  |  |  |

${ }^{\text {a }}$ B-spline CI with semi-empirical core potential (BCICP) method. ${ }^{102}$
${ }^{\mathrm{b}}$ MCHF method. ${ }^{1}$
${ }^{c} \mathrm{~B}$-spline CI (BCIBP) method. ${ }^{103}$


FIG. 1. The logarithmic map of calculated oscillator strengths for $S \rightarrow P$ and $P \rightarrow S$ transitions between states considered in this work.

TABLE 6. Comparison of the oscillator strength values for the $2^{1} S \rightarrow 2^{1} P$ transition in Be obtained with various experimental and theoretical approaches: Beam-foil (BF), Time-resolved laser-induced-fluorescence (TR-LIF), Time-dependent gauge invariant (TDGI), multiconfiguration Hartree-Fock (MCHF), B-spline Cl with semi-empirical core potential (BCICP), B -spline Cl ( BCIBP ), and $\mathrm{Cl}+$ core polarization (CICP)

| Experimental |  |
| :---: | :---: |
| $\mathrm{BF}^{104}$ | 1.34(4) |
| $\mathrm{BF}^{105}$ | 1.40(4) |
| TR-LIF ${ }^{106}$ | 1.34(3) |
| Theoretical |  |
| TDGI ${ }^{107,108}$ | 1.398 |
| BCICP ${ }^{102}$ | 1.375 |
| MCHF ${ }^{11}$ | 1.38 |
| BCIBP ${ }^{103}$ | 1.380 |
| CICP ${ }^{109}$ | 1.3743 |
| this work ( ${ }^{( } \mathrm{Be}$ ) | 1.3746892 (3) |
| this work ( ${ }^{9} \mathrm{Be}$ ) | 1.3744008 (3) |



FIG. 2. The density of the nucleus for some of the ${ }^{1} S$ (left-column) and ${ }^{1} P$ states (right-column) in the center-of-mass coordinate frame for the beryllium atom.


FIG. 3. The density of the electrons for some of the ${ }^{1} S$ (left-column) and ${ }^{1} P$ states (right-column) in the center-of-mass coordinate frame for the beryllium atom.
comparison. As can be seen, the FNM effects provide a significant contribution to the transition energies particularly for lower states. The transition energies calculated for ${ }^{9} \mathrm{Be}$ are in very good agreement with the experimental data available in the NIST Atomic Spectra Database (ver. 5.8). ${ }^{101}$ For the majority of states, the calculated transition-energy values are within the experimental error bars. However, there are states for which the discrepancies are slightly larger. These include, for example, the $9{ }^{1} P$ state. The origin of the discrepancies may be related to the way the experimental values were obtained. It is stated in the NIST ASD that the experimental energy levels for $n^{1} P(n=7-11)$ states listed there were determined by an extrapolation of the values obtained for the Rydberg states with lower $n$ 's using a quantum-defect expansion formula. However, it seems that this formula can only provide sound estimates of the energy levels for states with larger $n$. Upon a closer look at the transition energies involving state $9{ }^{1} P$, one finds that all experimental and the calculated results differ by about $10 \mathrm{~cm}^{-1}$. Such a consistent difference suggests that there may be a typographical error in the NIST ASD for the $9{ }^{1} P$ energy level.

In Table 5, we show the calculated values of the transition dipole moments and the oscillator strengths for ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$ for the $S \rightarrow P$ and $P \rightarrow S$ transitions involving all states considered in this work. The oscillator strengths are compared with available literature results. The oscillator strengths for all transitions considered in this work are shown in Fig. 1 in the form of a map that depicts their relative magnitude on a logarithmic scale.

In general, agreement between the oscillator strengths calculated in the present work and the available literature values is fairly good. The present calculations include a considerably wider range of the oscillator strength values than it was calculated in prior works. Both the tabulated values of the oscillator strengths and their depiction in Fig. 1 show that the largest values of the strengths correspond, as expected, to transitions between states with the same principal quantum number, i.e., $n^{1} S \rightarrow n^{1} P$ transitions. However, the oscillator strength values are also quite sizable for the $n^{1} P \rightarrow(n+1)^{1} S$ transitions. This indicates a possibility to use "cascade" excitations involving a sequence of the following transitions: $2{ }^{1} S \rightarrow 2{ }^{1} P, 2^{1}$ $P \rightarrow 3^{1} S, 3{ }^{1} S \rightarrow 3^{1} P, 3{ }^{1} P \rightarrow 4{ }^{1} S$, etc., to prepare the atom in a particular Rydberg state.

In Table 6, we provide a more detailed comparison of our oscillator strength values for the lowest $2{ }^{1} S \rightarrow 2{ }^{1} P$ transition with experimental and theoretical results from the literature. All theoretical values agree within the experimental uncertainties. It is interesting to note that there is a slight difference between the values of the oscillator strength calculated for ${ }^{9} \mathrm{Be}$ and ${ }^{\infty} \mathrm{Be}$ of 0.0003 . However, this isotopic shift is too small to be experimentally verifiable at present.

The finite-nuclear-mass effects can also be observed in the 3D plots of the radial electronic and nuclear densities determined with respect to the center of mass of the atom. The plots of these densities for some selected ${ }^{1} S$ and ${ }^{1} P$ states are shown in Figs. 2 and 3.

As one can see, with the increasing excitation level, the number of the radial nodes in the densities, as expected, increases. In addition, in the densities of the ${ }^{1} P$ states, there is a nodal plane along the $z$ plane. The most interesting is the comparison between the electronic and nuclear densities for a particular state. As one can see, the oscillatory patterns for the two densities for every state are almost
identical. However, the scale of the coordinate axes in the plots of the electronic densities is about four orders of magnitude larger than in the nuclear densities. As mentioned, this is understandable because the average radius of the motion of the nucleus around the center of mass of the atom is much smaller than the average radius of the motion of the electrons (the radius scales as the mass inverse). This also explains why the nodal patterns of the two densities for a particular state are very similar. This happens because, for each maximum of the nuclear density, a maximum of the electronic density has to appear to balance out the centrifuge effects associated with the motions of the particles. Due to this balance, the center of mass of the atom does not move.

## 4. Summary

In this work, an algorithm for calculating the oscillator strength for an atomic inter-state spectral transition is implemented and used to calculate the $S \rightarrow P$ and $P \rightarrow S$ transitions in the beryllium atom. In the calculations, the nonrelativistic variational wave functions expanded in terms of all-electron explicitly correlated Gaussian functions are used. In the calculation of the corresponding transition energies, the nonrelativistic energies are augmented with the leading relativistic and QED corrections and high-accuracy results are obtained. The nonrelativistic energies are the best to date. The oscillator strengths for the transitions show an interesting pattern. As the strength values are the most sizable for the $n^{1} S \rightarrow n^{1} P$ and $n^{1} P \rightarrow(n+1)^{1} S$ transitions, one can envision preparing a beryllium atoms in a particular excited Rydberg ${ }^{1} S$ or ${ }^{1} P$ state by a cascade of the following excitations: $2^{1} S \rightarrow 2{ }^{1} P, 2^{1} P \rightarrow 3{ }^{1} S, 3{ }^{1} S \rightarrow 3^{1} P$, etc. In moving back to the ground ${ }^{2} S$ state from a particular excited Rydberg ${ }^{1} S$ or ${ }^{1} P$ state, the above excitation cascade can be followed in reverse.

The present results may also be employed in the modeling of light emission and absorption events involving beryllium atoms in the interstellar media. Such models usually require accurate values of the transition energies and the oscillator strengths, which the present work provides.

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## 5. Data Availability

The data that support the findings of this study are available within the article and from the corresponding author upon reasonable request.

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