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 17 000 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.

CONTENTS

1.	Introduction	2
2.	Formalism	5
	2.1. Nonrelativistic nuclear-mass-dependent Hamiltonian	5
	2.2. Basis functions	e
	2.3. Relativistic and QED corrections	6
	2.4. Bethe logarithm fitting	7
	2.5. Oscillator strength	8
	2.6. Electronic and nuclear densities	8
3.	Results	9
4.	Summary	21
	Acknowledgments	21
5.	Data Availability	21
6.	References	21

List of Tables

Comparison of nonrelativistic energies of $^{\infty}$ 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-CI method (Hy-CI), 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).

4

8

10

14

18

19

- 2. Approximate values of the Bethe logarithm used in the calculations of the QED corrections for the lowest ten ¹S and ¹P states of beryllium.....
- 3. Convergence of the nonrelativistic energies (E_{nr}) , expectation values of the mass-velocity correction (H_{MV}) , δ -functions dependent on interparticle distances, principal value $\langle \mathscr{P}(1/r_{ij}^3) \rangle$, and total energies (E_{tot}) with the number of basis functions for the lowest ten ¹S and ¹P states of beryllium atom (⁹Be and [∞]Be).
- 5. The squares of the transition dipole moments, $|\mathbf{\mu}_{if}|^2$, and oscillator strengths, f_{iP} between ¹S and ¹P states....
- oscillator strengths, f_{if} between ¹S and ¹P states. 16
 Comparison of the oscillator strength values for the 2¹S → 2¹P 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 CI with semi-empirical core potential (BCICP), B-spline CI (BCIBP), and CI+ core polarization (CICP) 18

List of Figures

- 1. The logarithmic map of calculated oscillator strengths for $S \rightarrow P$ and $P \rightarrow S$ transitions between states considered in this work.
- 2. The density of the nucleus for some of the ¹S (left-column) and ¹P states (right-column) in the center-of-mass coordinate frame for the beryllium atom.
- 3. The density of the electrons for some of the ${}^{1}S$ (leftcolumn) and ${}^{1}P$ states (right-column) in the center-ofmass coordinate frame for the beryllium atom. 20

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 code¹⁰ and used it in their atomic oscillator-strength calculations. For the beryllium atom, oscillator-strength calculations were performed by Tachiev and Froese Fischer¹¹ using the aforementioned method. Their results were confirmed by Ynnerman and Froese Fischer¹² 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

J. Phys. Chem. Ref. Data **50**, 043107 (2021); doi: 10.1063/5.0065282 Published by AIP Publishing on behalf of the National Institute of Standards and Technology 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 ¹S and ¹P 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 ¹S states considered in Ref. 26 agreed with the experimental values to 0.02-0.09 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 $2s^{21}S_0 \rightarrow 2s2p^{-1}P_1$ transition has been calculated with rather high accuracy before. Puchalski *et al.*²³ used ECG to perform high-precision calculations of the $2s^{21}S_0 \rightarrow 2s2p^{-1}P_1$ transition energy and obtained the value of 42 565.441(11) 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 42 565.4501(13) 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 ⁹Be isotope of beryllium by Bozman et al.29 and the measurements of several beryllium transitions performed by Johansson.³⁰ The energy for the $2s^{2} S_0 \rightarrow 2s^2 p^{-1} P_1$ transition obtained in Johansson's experiment was 42 565.35(18) cm⁻¹. An important conclusion that emerged from comparing the calculated $2s^{21}S_0 \rightarrow 2s2p {}^1P_1$ 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 $2s^{2} {}^{1}S_{0} \rightarrow 2s2p {}^{1}P_{1}$ excitation energy determined by Puchalski et al. was equal to 1.048(9) 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 ¹S states and the ten lowest ¹*P* states of ⁹Be and $^{\infty}$ 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 non-relativistic 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 $^{\infty}$ 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-CI method (Hy-CI), 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

Work	Year	State	Method	Energy
Hartree and Hartree ³¹	1935	$2^{1}S$	HF	-14.57
Boys ³²	1950	$2^{1}S$	CI	-14.58
Rove ³³	1953	$2^{1}S$	PDVM	-14.637
boys		$2^{1}P$		-14.434
Brigman <i>et al.</i> ³⁴	1958	$2^{1}S$	CI	-14.5815
Watson ³⁵	1960	$2^{1}S$	CI	-14.65740
Weiss ³⁶	1961	$2^{1}S$	CI	-14.66090
Kelly ³⁷	1963	$2^{1}S$	MBPT	-14.663 11
Szasz and Byrne ³⁸	1967	$2^{1}S$	Hy	-14.6565
Gentner and Burke ³⁹	1968	$2^{1}S$	Hy	-14.6579
Bunge ⁴⁰	1968	$2^{1}S$	CI	-14.66419
Sims and Hagstrom ⁴¹	1971	$2^{1}S$	Hy-CI	-14.666547
Perkins ⁴²	1973	$2^{1}S$	Hy	-14.6611
Froese Fischer and Saxena ⁴³	1974	$2^{1}S$	MCHF	-14.665870
Bunge ⁴⁴	1976	$2^{1}S$	CI	-14.666902
Clementi et al.45	1991	$2^{1}S$	CI	-14.666 96
Mårtensson-Pendrill et al.46	1991	$2^{1}S$	MCHF	-14.66737
Davidson <i>et al.</i> ⁴⁷	1991	$2^{1}S$	EE	-14.66736
Froese Fischer ⁴⁸	1993	$2^{1}S$	MCHF	-14.667 113
Chakravorty et al.49	1993	$2^{1}S$	EE	-14.66736
Komasa <i>et al.</i> ⁵⁰	1995	$2^{1}S$	ECG	-14.667360(2)
Noga <i>et al.</i> ⁵¹	1995	$2^{1}S$	CCSDT1-R12	-14.667 261
Jitrik and Bunge ⁵²	1997	$2^{1}S$	CI	-14.667 275 57
Busse and Lüchow ⁵³	1997	$2^{1}S$	Hy	-14.667 354 7
	2001	$2^{1}S$	ECG	-14.667 355 536
Komasa ⁵⁴		2 P		-14.47344433
Komasa		$3^{1}P$		-14.393 113 93
		$4 \ ^{1}P$		-14.361 789 21
Pachucki and Komasa ⁵⁵	2004	$2^{1}S$	ECG	-14.667 355 627
Pachucki and Komasa ⁵⁶	2006	$2^{1}S$	ECG	-14.667 355 748
Nakatsuji <i>et al.</i> ⁵⁷	2007	$2^{1}S$	LSE-ICI	-14.667300
Toulouse and Umrigar ⁵⁸	2008	$2^{1}S$	DMC	-14.66727(1)
	2009	$2^{1}S$	ECG	-14.667356486
		$3^{1}S$		-14.418240328
Stanke <i>et al</i> . ²⁴		$4^{1}S$		-14.370087876
		$5^{1}S$		-14.351 511 654
		6 ¹ S		-14.342403552
Verdebout et al.59	2010	$2^{1}S$	MCHF	-14.66711452
Bunge ⁶⁰	2010	$2^{1}S$	CI	-14.667355(1)
King <i>et al.</i> ⁶¹	2011	$2^{1}S$	Hy	-14.667 02
Sims and Hagstrom ⁶²	2011	$2^{1}S$	Hy-CI	-14.667 356 411
Komasa <i>et al.</i> ⁶³	2013	$2^{1}S$	ECG	-14.667 356 4
Puchalaki at al^{23}	2013	$2^{1}S$	ECG	-14.667 356 498
r uchalski et al.		2 ¹ <i>P</i>		-14.473451370

Work	Year	State	Method	Energy
Sharma <i>et al.</i> ⁶⁴	2014	2 ¹ S	DMRG	-14.667 207
Sims and Hagstrom ⁶⁵	2014	$2^{1}S$	Hy-CI	-14.667 356 407 951
C C	2014	$2^{1}P$	ECG	-14.473451378
		$3^{1}P$		-14.393 143 528
		$4 \ ^{1}P$		-14.361 938 388
Bubin and Adamowicz ⁶⁶		5 P		-14.347876275
		6 P		-14.340470145
		7 P		-14.336 115 562
		$8 \ ^{1}P$		-14.333344814
Przybytek and Lesiuk ⁶⁷	2018	$2^{1}S$	ECFCC	-14.667 351
	2019	$2^{1}S$	ECG	-14.667356508(1)
Hornvák at al 26		$3^{1}S$		-14.418240368(2)
Homyak et ul.		$4^{1}S$		-14.370087938(4)
		5 ¹ S		-14.351 511 736(7)
	2019	$2^{1}P$	ECG	-14.4734513882
		$3^{1}P$		-14.393 143 5385
		$4 \ ^{1}P$		-14.361 938 3998
		5 P		-14.3478762953
Stanke <i>et al.</i> ²⁷		6 P		-14.3404701944
		7 P		-14.3361157060
		$8 \ ^{1}P$		-14.3333453168
		$9^{1}P$		-14.3314759537
		$10 \ ^{1}P$		-14.3301549127
		$11 \ ^{1}P$		-14.3291852411
Nasiri and Zahedi ⁶⁸	2020	$2^{1}S$	DMC	-14.66734(5)
	2020	3 ¹ S	Hy-CI	-14.418240346
		$4^{1}S$		-14.370087890
Sims ⁶⁹		$5^{1}S$		-14.351 511 676
		6 ¹ S		-14.342403578
		$7^{1}S$		-14.337266500

TABLE 1. (Continued)

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 3N - 3 = 3n "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, ..., 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_{CM} , Y_{CM} , and Z_{CM} and the internal coordinates, \mathbf{r}_i , i = 1, ..., 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, ..., n coordinates and has the following form (atomic units are assumed throughout):

$$H_{\rm nr}^{\rm int} = -\frac{1}{2} \left(\sum_{i=1}^{n} \frac{1}{\mu_i} \nabla_{\mathbf{r}_i}^2 + \sum_{i=1}^{n} \sum_{j \neq i}^{n} \frac{1}{m_0} \nabla_{\mathbf{r}_i}' \nabla_{\mathbf{r}_j} \right) + \sum_{i=1}^{n} \frac{q_0 q_i}{r_i} + \sum_{i=1}^{n} \sum_{j < i}^{n} \frac{q_i q_j}{r_{ij}},\tag{1}$$

where q_0 is charge of the nucleus, $q_i = -1(i = 1, ..., n)$ are the electron charges, m_0 is the nuclear mass ($m_0 = 16\ 424.2055m_e$ for ⁹Be), $m_i = 1$ are the electron masses, $\mu_i = m_0 m_i / (m_0 + m_i)$ is the reduced mass of electron *i*, r_i is the distance between the nucleus and electron *i*, and $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$ is the distance between electrons *i* and *j*. In this work, we use the following ⁹Be nuclear mass: $m_0(^9Be) = 16\ 424.2055m_e,^{70}$ where m_e is the mass of the electron. By setting m_0 to infinity in H_{nr}^{int} , one gets the INM Hamiltonian that is used in the standard calculations based on the Born–Oppenheimer approximation. Both FNM and INM 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 form⁷¹

$$H_{\rm nr}^{\rm int} = -\nabla_{\mathbf{r}}' \mathbf{M} \nabla_{\mathbf{r}} + \sum_{i=1}^{n} \frac{q_0 q_i}{\mathbf{r}_i} + \sum_{i=1}^{n} \sum_{j < i}^{n} \frac{q_i q_j}{\mathbf{r}_{ij}},\tag{2}$$

where

$$\nabla_{\mathbf{r}} = \begin{pmatrix} \nabla_{\mathbf{r}_1} \\ \vdots \\ \nabla_{\mathbf{r}_n} \end{pmatrix}$$

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 3×3 identity matrix I_3 . Matrix M has diagonal elements $1/(2\mu_1), \ldots,$ and $1/(2\mu_n)$, while all off-diagonal elements are equal to $1/(2m_0)$. 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:

$$\phi_k = \exp\left[-\mathbf{r}'(A_k \otimes I_3)\mathbf{r}\right],\tag{3}$$

where A_k is an $n \times n$ real symmetric matrix, \otimes is the Kronecker product, and I_3 is a 3×3 identity matrix. The *P*-type Gaussians have the following form:

$$\phi_k = z_{i_k} \exp\left[-\mathbf{r}'(A_k \otimes I_3)\mathbf{r}\right],\tag{4}$$

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, ..., n) range and is an adjustable parameter in our calculations. The parameter is specific for each

basis function, ϕ_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 $A_k = L_k L'_k$, 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 constraints from $-\infty$ to ∞ . 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 $Y = (1 - P_{13})(1 - P_{24})(1 + P_{12})(1 + P_{34})$, where P_{ij} 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 ⁹Be isotope and then reused in the $^{\infty}$ 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, α .^{76,77} The first term in this expansion is the nonrelativistic energy of the considered state, E_{nr} ,

$$E_{\rm tot} = E_{\rm nr} + \alpha^2 E_{\rm rel}^{(2)} + \alpha^3 E_{\rm QED}^{(3)} + \alpha^4 E_{\rm HQED}^{(4)} + \cdots,$$
 (5)

the second term, $\alpha^2 E_{\rm rel}^{(2)}$, represents the leading relativistic corrections, the third term, $\alpha^3 E_{\rm QED}^{(3)}$, represents the leading QED corrections, and the fourth term, $\alpha^4 E_{\rm HQED}^{(4)}$, 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 $\alpha^2 E_{\rm rel}^{(2)}$ term is calculated as the expectation value of the Dirac–Breit Hamiltonian in the Pauli approximation, $H_{\rm rel}$.^{78,79} In the present calculations of the ¹S and ¹P states of beryllium, the Hamiltonian for the relativistic correction, $H_{\rm rel}$, contains the following terms:

$$H_{\rm rel} = H_{\rm MV} + H_{\rm D} + H_{\rm OO} + H_{\rm SS},\tag{6}$$

where operators $H_{\rm MV}$, $H_{\rm D}$, $H_{\rm OO}$, and $H_{\rm SS}$ 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, ..., 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 $\alpha^3 E_{\text{QED}}^{(3)}$ 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:

$$H_{\text{QED}}^{(3)} = \sum_{\substack{i,j=1\\j>i}}^{n} \left[\left(\frac{164}{15} + \frac{14}{3} \ln \alpha \right) \delta(\mathbf{r}_{ij}) - \frac{7}{6\pi} \mathscr{P} \left(\frac{1}{r_{ij}^3} \right) \right] \\ + \sum_{i=1}^{n} \left(\frac{19}{30} - 2 \ln \alpha - \ln k_0 \right) \frac{4q_0}{3} \delta(\mathbf{r}_i), \tag{7}$$

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

$$\left(\mathscr{P}\left(\frac{1}{r_{ij}^3}\right)\right) = \lim_{a \to 0} \left(\frac{1}{r_{ij}^3}\Theta(r_{ij}-a) + 4\pi(\gamma + \ln a)\delta(\mathbf{r}_{ij})\right).$$
(8)

Here, $\Theta(\cdots)$ is the Heaviside step function and $\gamma = 0.577\ 215\ldots$ is the Euler–Mascheroni constant.

The last term in $H_{\text{QED}}^{(3)}$ 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 $E_{\text{HQED}}^{(4)}$ term. It can be calculated as the expectation value of the following approximate operator derived by Pachucki *et al.*:^{55,85}

$$H_{\rm HQED}^{(4)} = \pi q_0^2 \left(\frac{427}{96} - 2 \ln 2\right) \sum_{i=1}^n \delta(\mathbf{r}_i).$$
(9)

 $E_{\rm HQED}^{(4)}$ 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 $E_{\rm HQED}^{(4)}$ for light atoms with the overall error being of the order of 50%.

The expectation values of the $H_{\rm QED}^{(3)}$ and $H_{\rm HQED}^{(4)}$ 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 $E_{\rm QED}^{(3)}$ and $E_{\rm HQED}^{(4)}$ 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 $\nabla_{\mathbf{r}}^4$ operator in $H_{\rm MV}$ and the one- and two-electron Dirac delta functions, $\delta(\mathbf{r}_i)$ and $\delta(\mathbf{r}_{ij})$, in H_D , H_{SS} , H_{QED} , and H_{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 Drachman⁹¹ 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 $\delta(\mathbf{r}_i)$, $\delta(\mathbf{r}_{ij})$, 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 (2¹S, 2¹P, and 3¹S) 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 Goldman⁹³ showed that the value of the Bethe logarithm for atomic Rydberg states has

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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 $S(2 \ ^1S, 3 \ ^1S)$ and $P(2 \ ^1P)$ states of the Be atom. In our fitting, the Bethe logarithm value for the ground 2^2S state of Be⁺ ion⁹⁴ is used as the asymptotic value when $n \to \infty$. 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 ground-state 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_{if} for a transition between an initial state *i* and a final state *f* is defined as^{95,96}

$$f_{if} = \frac{2}{3g_i} \left(\frac{Z_r}{Z_p}\right) \Delta E_{if} |\langle \psi_i | \boldsymbol{\mu} | \psi_f \rangle|^2, \qquad (10)$$

where $g_i = 2J_i + 1$ is the statistical weight of the lower level, $\Delta E_{if} = |E_i - E_f|$ is the transition energy, $Z_r = \frac{q_0 m_e + m_0}{nm_e + m_0}$ 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 μ is the electric dipole-moment operator. For an atom containing n electrons, $\mu = \sum_{i=1}^{n} q_i \mathbf{r}_i$, 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 ¹S and ¹P states of beryllium. All values are in atomic units

State	Reference	$\ln k_0$	$\ln(k_0/q_0^2)$
2 ¹ S	4	5.750 46	2.977 871
3 ¹ S	4	5.751 49	2.978 901
$4^{1}S$		5.751 698	2.979 109
5 ¹ S		5.751 783	2.979 195
6 ¹ S		5.751 821	2.979 232
7 ¹ S		5.751 840	2.979 252
8 ¹ S		5.751 851	2.979 262
9 ¹ S		5.751 858	2.979 269
$10^{1}S$		5.751 862	2.979 273
11 ¹ S		5.751 865	2.979 276
$2^{1}P$	4	5.752 320	2.979 731
$3^{1}P$		5.751 989	2.979 401
$4 {}^{1}P$		5.751 909	2.979 320
$5 {}^{1}P$		5.751 880	2.979 291
$6 {}^{1}P$		5.751 867	2.979 279
7 P		5.751 861	2.979 272
8 ¹ P		5.751 857	2.979 269
9 ¹ <i>P</i>		5.751 855	2.979 266
$10^{-1}P$		5.751 854	2.979 265
$11 \ ^1P$		5.751 853	2.979 264
$2^2 S Be^+$	94	5.751 849	2.979 260
$1^2 S H$	93	2.984 128	2.984 128

system, respectively. Wave functions ψ_i and ψ_f are nonrelativistic wave functions obtained in variational calculations using Hamiltonian (2). As the Hamiltonian explicitly depends on the mass of the nucleus, ψ_i and ψ_f also depend on the nuclear mass, i.e., they are slightly different for ⁹Be and [∞]Be. It is worth mentioning that for a charge-neutral system, μ 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:

$$|\mu_{if}|^{2} = |\langle \psi_{i} | \boldsymbol{\mu} | \psi_{f} \rangle|^{2} = |\langle \psi_{i} | \mu_{x} | \psi_{f} \rangle|^{2} + |\langle \psi_{i} | \mu_{y} | \psi_{f} \rangle|^{2} + |\langle \psi_{i} | \mu_{z} | \psi_{f} \rangle|^{2}.$$
(11)

For oscillator strengths, only the transition dipole moments between the $S(L = 0, M_L = 0)$ and $P(L = 1, M_L = 0)$ 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 $S(L = 0, M_L = 0)$ and $P(L = 1, M_L = 0)$ 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 $S(L = 0, M_L = 0)$ and $P(L = 1, M_L = 0)$ ECGs can be expressed as

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

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 $\boldsymbol{\varepsilon}^{z'} \equiv (0, 0, 1)$. 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 ,

$$\tilde{\mathbf{A}}_k = \mathbf{P}'_k \mathbf{A}_k \mathbf{P}_k, \quad \tilde{\mathbf{A}}_l = \mathbf{P}'_l \mathbf{A}_l \mathbf{P}_l, \quad \tilde{\mathbf{v}}^l = \mathbf{P}'_l \mathbf{v}^l, \quad z_{\tilde{m}_k} = \tilde{\mathbf{v}}^l \mathbf{r}$$

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

$$\left\langle \tilde{\phi}_{k}^{(0)} \middle| z_{l} \middle| \tilde{\phi}_{l}^{(1)} \right\rangle = \frac{\pi^{\frac{3\pi}{2}}}{2} \frac{\nu^{\prime\prime} \tilde{A}_{kl}^{-1} \tilde{\nu}^{l}}{\left| \tilde{A}_{kl} \right|^{\frac{3}{2}}},$$
(13)

where $\tilde{A}_{kl} = \tilde{A}_k + \tilde{A}_l$.

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2.6. Electronic and nuclear densities

The density of particle *i* in the center-of-mass (COM) coordinate frame is defined as $\rho_i(\boldsymbol{\xi}) = \langle \delta(\mathbf{R}_i - \mathbf{R}_{cm} - \boldsymbol{\xi}) \rangle$, where i = 1, ..., N and \mathbf{R}_{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 ×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 ${}^{9}Be$ isotope, i.e., the FNM Hamiltonian (2) is used. The basis sets are

subsequently used in the calculations for $^{\infty}$ Be. The nonrelativistic energies are shown in Table 3. The results for the ⁹Be isotope and for $^{\infty}$ Be are shown as well. For each ^{1}S and ^{1}P state of 9 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 $^{\infty}$ 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 ⁹Be. These energies are compared with the best previously published results. Our largest basis sets range from 16 000 basis functions for the lower states to 17 000 for the top states. For all states, the values of the nonrelativistic ⁹Be and $^{\circ}$ Be energies are notably lower than the values previously reported in the literature. For example, for the ground ¹S state, the present energy value of $^{\infty}$ Be, -14.667 356 508 8 a.u., is lower than the value of -14.667 356 498(3) a.u. reported in 2013 by Puchalski et al.²³ by about 1×10^{-8} a.u. For the lowest ${}^{1}P$ state, the analogous comparison is -14.473 451 389 5 a.u. (our present value) and -14.473 451 37(4) a.u. (the value of Puchalski et al.23). Another example concerns our previous calculations of the five lowest ¹S states.²⁶ The ⁹Be and [∞]Be energies obtained in that work with 7000 ECGs for the ground state are -14.666 435 525 and -14.667 356 507 a.u., respectively, while the corresponding values obtained in the present calculations are -14.6664355264 and -14.6673565084 a.u., respectively. For 5 ¹S, the corresponding comparison is -14.350 610 425 9 and -14.351 511 733 9 a.u. (the present calculations) and -14.350 610 414 and -14.351 511 722 in the calculations of Hornyák et al.²⁶ As one can notice, the improvement is larger for 5 ¹S than for the 2 ¹S 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 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 ⁹Be and $^{\infty}$ 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, $\langle H_{\rm MV} \rangle$, the orbit-orbit correction, $\langle H_{\rm OO} \rangle$, and the oneand two-electron δ -functions [$\langle \delta(\mathbf{r}_i) \rangle$ and $\langle \delta(\mathbf{r}_{ij}) \rangle$ respectively]. The $\langle \mathscr{P}(1/r_{ii}^3) \rangle$ expectation value is also shown. For the ⁹Be isotope, the results obtained using basis sets with different numbers of ECGs are shown to assess the convergence. For $^{\infty}$ 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, $E_{\rm tot}$, 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_{tot} values are used to calculate the interstate transition energies.

The $S \rightarrow P$ and $P \rightarrow S$ transition energies for ⁹Be and [∞]Be calculated using E_{tot} values taken from Table 3 are shown in Table 4. The values derived from experimental data are also included for

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TABLE 3. Coenergies (EtThe tilde sign	onvergence (ot) with the n indicates th	of the nonrelati number of basis at expectation	vistic energies ($E_{\rm nr}$), expectati functions for the lowest ten 1S value identities were employed	on values of the mas and ¹ <i>P</i> states of bery to compute the corres	s-velocity correction ($_{\rm 0}$ llium atom ($_{\rm 9}$ Be and $^\infty$ sponding quantities to	H _{MV}), <i>δ</i> -functions depe Be). The numbers in pe improve their converger	indent on interparticle trentheses are estimal toe. All values are in a	distances, principal ve ted uncertainties due to tomic units	alue $\langle \mathscr{P}(1/r_{j}^{3}) \rangle$, and total the basis truncation error.
State Isoto	pe Basis	Reference	Enr	$\langle ilde{H}_{\mathrm{MV}} angle$	$\langle H_{00} \rangle$	$\langle ilde{\delta}(\mathbf{r}_i) angle$	$\langle ilde{\delta}(\mathbf{r}_{ij}) angle$	$\langle \mathscr{P}(1/r_{ij}^3) angle$	$E_{ m tot}$
B B	$\begin{array}{ccc} 14.00 \\ 15.00 \\ 16.00 \\ 16.00 \\ 5e \\ 7.000 \end{array}$	00 00 00 26	-14.666 435 525 2 -14.666 435 526 1 -14.666 435 526 4 -14.666 435 526 4 -14.666 435 526 8(2) -14.666 435 525	-270.636 666 -270.636 645 -270.636 556 -270.636 510	-0.91846159 -0.91846158 -0.91846157 -0.91846157	8.840 617 349 8.840 617 352 8.840 617 354 8.840 617 354 8.840 617 34	0.267 506 284 0.267 506 285 0.267 506 286 0.267 506 284 0.267 506 284	-1.222 66 -1.222 43 -1.221 35	-14.668 440 604 -14.668 440 604 -14.668 440 604 -14.66 844 059 7(18)
2 ¹ S °	3e 7 000	00 26 0 4 26 26	$\begin{array}{c} -14.666435526(1)\\ -14.6673565084\\ -14.6673565087(2)\\ -14.667356498(3)\\ -14.667356507\\ -14.667356507\\ -14.667356508(1)\end{array}$	-270.703 526 -270.703 76(11) -270.703 579	-0.89182369 -0.89182410(8) -0.89182362	8.842 251 649 8.842 250 65(15) 8.842 251 64	0.267 550 917 0.267 550 888 (15 0.267 550 915	-1.22178)-1.2211277(5) -1.22252	-14.669 361 498 -14.669 361 494(18)
^{9}E	14 60 15 50 3e 16 40 0 0 16 40 16 40 16 40 3e ∞	00 00 00 27 00 27	$\begin{array}{c} -14.4725437569\\ -14.4725437577\\ -14.472543761(19)\\ -14.4725437647(19)\\ -14.4725437598\\ -14.4734513895\\ -14.4734513933(19)\\ -14.4734513933(19)\\ -14.4734513882\end{array}$	-266.598 045 -266.598 039 -266.598 021 -266.664 445 -266.665 14(15)	-0.838 224 67 -0.838 224 67 -0.838 224 64 -0.838 224 6 -0.838 224 6 -0.812 091 50 -0.812 092 9(3) -0.812 091 5	8.722 853 523 8.722 853 527 8.722 853 539 8.724 481 450 8.724 478 65(20)	0.261 279 705 0.261 279 705 0.261 279 707 0.261 324 034 0.261 323 93(3)	-1.18489 -1.18483 -1.18462 -1.18506 -1.182858(13)	-14.474 498 170 -14.474 498 170 -14.474 498 173 -14.474 498 175 (13) -14.475 405 724 -14.475 405 726(13)
3 ¹ S	14 00 15 00 15 00 7 000 7 000 3e 7 000	00 00 00 26 0 26 26 26 26	$\begin{array}{c} -14.417\ 335\ 140\ 0\\ -14.417\ 335\ 142\ 9\\ -14.417\ 335\ 142\ 5\\ -14.417\ 335\ 143\ 5\\ -14.417\ 335\ 143\ 1(6)\\ -14.418\ 335\ 139\\ -14.418\ 235\ 139\\ -14.418\ 240\ 368\ 2\\ -14.418\ 240\ 368\ 2\\ -14.418\ 240\ 368\ 2\\ -14.418\ 240\ 368\ 2\\ \end{array}$	-268.474 994 -268.474 893 -268.474 803 -268.474 926 -268.541 128 -268.541 251	$\begin{array}{c} -0.92653944\\ -0.92653939\\ -0.92653937\\ -0.92653941\\ -0.90012850\\ -0.90012850\\ -0.90012821\end{array}$	8.780 376 771 8.780 376 781 8.780 376 790 8.780 376 76 8.781 996 527 8.781 996 50	0.263 820 372 0.263 820 375 0.263 820 377 0.263 820 371 0.263 864 254 0.263 864 254	-1.248 41 -1.247 36 -1.246 34 -1.246 77 -1.248 22	-14.419 312 274 -14.419 312 272 -14.419 312 269 -14.419 312 265(19) -14.420 217 407 -14.420 217 403(19)
$3^{1}P$ $^{\circ}F$	14 60 15 50 16 40 16 40 16 40 3e ∞ 3e ∞	00 00 00 27 00 27	$\begin{array}{c} -14.392\ 242\ 880\ 3\\ -14.392\ 242\ 881\ 8\\ -14.392\ 242\ 886\ 1\\ -14.392\ 242\ 886\ 1\\ -14.392\ 242\ 884\ 4\\ -14.392\ 143\ 540\ 2\\ -14.393\ 143\ 544\ 6(22)\\ -14.393\ 143\ 538\ 5\\ \end{array}$	-267.390 569 -267.390 566 -267.390 546 -267.456 802	$\begin{array}{c} -0.88208043\\ -0.88208043\\ -0.88208040\\ -0.88208040\\ -0.85581150\\ -0.85581150\\ -0.85581150\end{array}$	8.747 804 857 8.747 804 867 8.747 804 893 8.749 425 262	$0.262\ 237\ 919$ $0.262\ 237\ 920$ $0.262\ 237\ 922$ $0.262\ 281\ 844$	-1.227 10 -1.227 07 -1.226 80 -1.226 80	-14.394206423 -14.394206424 -14.394206427 -14.394206431(17) -14.395106998 -14.395107001(17)

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Journal of Physical and Chemical Reference Data

TABLE	3. (Continuea									
State	Isotope	Basis	Reference	$E_{ m nr}$	$\langle ilde{H}_{ m MV} angle$	$\langle H_{\rm OO} \rangle$	$\langle ilde{\delta}(\mathbf{r}_i) angle$	$\langle ilde{\delta}({f r}_{ij}) angle$	$\langle \mathscr{P}(1/r_{ij}^3) angle$	$E_{ m tot}$
		14 000 15 000		$-14.369\ 185\ 505\ 1$ $-14\ 369\ 185\ 510\ 9$	-268.315 505 -268 315 475	-0.932 337 62 -0 932 337 58	8.776 228 493 8 776 228 516	0.263 512 821 0 263 512 824	-1.25293 -175749	-14.371 60 487 -14 371 160 492
	9 Be	16 000		-14.369 185 512 9 14.360 186 512 9	-268.315411	-0.932 337 56	8.776 228 530	0.263 512 826	-1.251 82	-14.371 160 491
, 1c		7 000	26	-14.369 185 506	-268.315685	-0.932 337 71	8.776 228 47	0.263 512 813		(01) CZF 001 1 /C'F1 -
4 0		~ 16 000	26	$-14.369\ 185\ 514(4)$ $-14\ 370\ 087\ 936\ 7$	-768 381 663	-0 905 938 87	8 777 846 410	0 263 556 605	-1 252 25	-14 377 067 878
	° Be	8		$-14.370\ 087\ 939\ 7(15)$		10 000 00000	011 010 ///0		- 1.474 40	-14.372062830(10)
		7 000 ~	26 26	$-14.370\ 087\ 930$ $-14.370\ 087\ 938(4)$	-268.381 937	-0.905 938 65	8.777 84635	0.263 556 591	-1.25516	
		14 600 15 500		-14.361 037 794 6 -14 361 037 796 1	-267.893328 -767 803377	-0.913 549 58	8.763 470 236 8 763 470 248	0.262 900 115	-1.244 68 -1 244 63	-14.363 007 512 -14 363 007 513
	^{9}Be	16 400		$-14.361\ 037\ 802\ 2$	-267.893 223	-0.91354952	8.763 470 279	0.262 900 121	-1.24349	-14.363007515
$4^{1}P$		8		$-14.361\ 037\ 808\ 6(36)$						-14.363007517(9)
•		16 400 16 400	27	-14.361 037 799 9 -14 361 038 402 2	-767 959 411	-0.913 549 5 -0 887 204 01	8 765 087 777	298 200 292 0	-1 243 92	-14 363 908 078
	$^{\circ}{ m Be}$	07E 01		-14.3619384094(36)	TTE / C/ 107	10 107 /000	7 /7 /00 /0 /0	100 CE/ 707.0	7/ 617.1	-14.363908030(9)
		16400	27	-14.361 938 399 8		$-0.887\ 204\ 0$				
		14 000		-14.350 610 4118	-268.272 968	-0.93416435	8.775 161 626	0.263 430 584	-1.25427	-14.352 584 783
		15000		-14.3506104247	-268.272868	-0.93416426	8.775 161 679	$0.263\ 430\ 591$	-1.25307	-14.352584791
	⁹ В.е	$16\ 000$		-14.3506104259	-268.272870	-0.93416426	8.775 161 683	$0.263\ 430\ 592$	-1.25306	-14.352584793
	2	8		-14.3506104274(8)						-14.352584795(11)
$5^{1}S$		7 000	26 26	-14.350610414	-268.273164	-0.934 164 45	8.775 161 59	0.263430571	-1.25516	
		16 000	07	$-14.350\ 010\ 420(7)$	-268 339 105	-0 907 768 57	8 776 779 118	0 263 474 347	-1.253.49	$-14\ 353\ 486\ 014$
	о СС 8	8		-14.3515117354(8)						-14.353486015(11)
	be	7 000	26	-14.351511722	-268.339399	-0.90776818	8.77677903	0.263474325	-1.25659	~
		8	26	-14.351511736(7)						
		14 600		-14.3469758541	-268.071039	-0.92493225	8.769 034 122	0.263 137 388	-1.252 92	-14.348947726
	-0	15 500		-14.346 975 8568	-268.071032	-0.92493223	8.769 034 146	0.263 137 390	-1.25284	-14.348947729
	, Be	16400		-14.346 9/5 86/ 2 -14 346 075 878 4/56)	686.0/0.892-	-0.924 932 17	8.769 034 198	0.263 137 397	-1.252 35	-14.348 947 737 -14 348 947 745742)
$5^{1}P$		16400	27	-14.346 975 863 8		-0.9249322				(77)(74)/14/04(77)/
		16400		-14.3478762988	-268.137180	-0.898 561 42	8.770 650 913	0.263 181 123	-1.25278	-14.349848081
	° Be	$\stackrel{\infty}{16400}$	27	-14.3478763100(56) -14.3478762953		-0.898 561 4				-14.349848090(42)
		$14\ 000$		-14.3415028839	-268.257 684	-0.93492953	8.774 781 459	0.263 400 264	-1.258 15	-14.343477035
	⁹ Be	15000		-14.3415029126	-268.257307	-0.93492921	8.774 781 652	0.263400285	-1.25490	-14.343477046
6 ¹ S	S	16 000		-14.341 502 922 5	-268.257223	-0.934 929 13	8.774 781 679	0.263400291	-1.25412	-14.343 477 052
	8	$16\ 000$		-14.342 403 676 6	-268.323 452	-0.90853440	8.776 399 001	0.263 444 038	-1.25455	-14.3443777719
	pe	8		-14.3424036918(53)						-14.344377725(36)

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J. Phys. Chem. Ref. Data 50, 043107 (2021); doi: 10.1063/5.0065282

	3. (Continue	a)								
State	Isotope	Basis	Reference	$E_{ m nr}$	$\langle \tilde{H}_{\mathrm{MV}} \rangle$	$\langle H_{00} \rangle$	$\langle ilde{\delta}(\mathbf{r}_i) angle$	$\langle ilde{\delta}(\mathbf{r}_{ij}) angle$	$\langle \mathscr{P}(1/r_{ij}^3) angle$	$E_{ m tot}$
		$14\ 600$ $15\ 500$		-14.3395698970 -14.3395699048	-268.147 264 -268.147 262	-0.92983934 -0.92983927	8.771 437 062 8.771 371 04	$0.263\ 240\ 458$ $0.263\ 240\ 462$	-1.25408 -1.25405	-14.341542673 -14.341542680
	$^9\mathrm{Be}$	16 400		-14.339 569 932 7	-268.147115	-0.92983912	8.771 437 280	0.263 240 478	-1.25223	-14.341542702
$6^{1}P$		000 16 400	70	-14.339569964(15) -14.339569964(15)		_0 070 830 3				-14.34154273(12)
		16 400	4	-14.3404702036	-268.213318	-0.90345780	8.773 054 048	0.263 284 203	-1.25266	-14.342442886
	°Be	\sim 16 400	27	-14.340470233(15) -14.340470194		-0.9034578				-14.34244291(12)
		14 000		-14.3363659009	-268.251719	-0.935 320 56	8.774 622 594	0.263 386 930	-1.26545	-14.338 339 983
	9 ₀ 0	15 000		-14.3363660542	-268.251428	-0.93531972	8.774 623 708	0.263 387 016	-1.26235	-14.338340121
$7^{1}S$	DG	$16\ 000$		-14.3363660919	-268.251 267	-0.93531938	8.774 623 968	$0.263\ 387\ 047$	-1.26089	-14.338340151
)	о ⁰ 0	$^{\infty}_{16\ 000}$		-14.336366132(20) -14.3372665320	-268.317 496	-0.90892495	8.776 241 280	0.263 430 793	-1.26132	-14.33834018(15) -14.339240504
	DC	8		-14.337266572(20)						-14.33924054(15)
		14600		-14.3352154669	-268.185790	-0.93228661	8.772 641 931	$0.263\ 292\ 332$	-1.25824	-14.337188708
	,	15500		-14.3352154836	-268.185794	-0.93228655	8.772 642 041	$0.263\ 292\ 336$	-1.25821	-14.337188725
	$^{9}\mathrm{Be}$	16400		-14.3352155735	-268.185654	-0.932 286 11	8.772 642 568	$0.263\ 292\ 395$	-1.25595	-14.337188808
$7^{1}P$		8	Ĩ	-14.335215667(50)						-14.33718889(42)
		16 400	27	-14.3352155592	268 251 862	-0.9322865 0.00580050	0 111 250 120		1 257 20	11 338 088 860
	о ^д ∞	10 400		-14.330115/211 14.330115 020/60	COQ 1 C7 QO7-	UC 668 CU6.U-	0.1/4 209 420	771 000 007.0	00007.1-	-14.330 000 009 14 220 000 05/47)
	De	16400	27	-14.336115706		-0.9058997				(74)066 000 000.47
		00011								
		15 000		-14.333 185 490 / 14 222 185 750 0	-268.248468	19 066 686.0- 12 063 300 0	005 155 4/7.8	0.263 380 462	-17 C2C 1	-14.335 155 VCI 750 027 031 300 VI
	$^{9}\mathrm{Be}$	000 71		0 6C / COI CCC.+1- 2 20 201 00 105 005	-200.24/ 932 260 717 002	10 645 556.0-	0.0 200 4/70 0.00	0.00.000 200.00/ 0.02 200.772	-1.20241 1.260.05	00/60100071-
8 ¹ S		000 0T		-14.33318626(16)	-200.241 900	10 040 006.0-	070 700 700 100	C7 / NOC CO7.N	CU U02.1-	-14.3351603(15)
		16 000		14.334 086 751 0	-768 311 713	-0 000 157 40	021 221 922 8	0 763 474 460	-1 760.48	14.336 060 164
	°Be	8		-14.33408656(16)	C17 & 1C'007-	67 FCI 606.0-	0/17/10//0	201 171 CO7.0	040071-	-14.3360604(15)
		14600		-14.3324449402	-268.207584	-0.93364105	8.773 310 065	0.263 321 187	-1.26504	-14.334418458
	-0	15 500		-14.3324450069	-268.207 593	-0.93364086	8.773 310 409	0.263 321 197	-1.26488	-14.334418525
	Be	16 400		-14.3324453165	-268.207487	-0.93364032	8.773 312 276	0.263 321 319	-1.26184	-14.334418 829
$8^{1}P$		∞ 16 400	27	-14.33244503(20) -14.3324452635		-0.9336411				-14.3344191(1/)
		16 400	i	-14.3333453727	-268.273702	-0.90725064	8.774 929 236	$0.263\ 365\ 049$	-1.26228	-14.335318798
	∞Be	8		-14.33334577(20)						-14.3353191(17)
		$16\ 400$	27	-14.3333453168		-0.9072510				
		15 000		-14.3310804172	-268.245947	-0.93570483	8.774 517 184	0.263 376 905	-1.27061	-14.333054364
	9 RA	$16\ 000$		-14.3310806115	-268.246125	-0.93570450	8.774 519 513	$0.263\ 377\ 024$	-1.26988	-14.333054565
9 ¹ S	S	17 000		-14.3310808174	-268.246315	-0.93570387	8.774 521 837	$0.263\ 377\ 150$	-1.26907	-14.333054778
		000 17 000		-14.331 U81 18(18) -14 331 980 933 9	-768 317 545	-0 909 308 87	8 776 139 224	0 263 420 896	-1 26951	-14.33305205(28)
	°Be	8		-14.33198133(18)	CEC 710.007	00000000	177 / / / / / / /	0/0 075 007.0	10/07:1	-14.3339551(28)

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TABLE 3	t. (Continuea	<u> </u>								
State	Isotope	Basis	Reference	$E_{ m nr}$	$\langle ilde{H}_{ m MV} angle$	$\langle H_{\rm OO} \rangle$	$\langle ilde{\delta}(\mathbf{r}_i) angle$	$\langle ilde{\delta}({f r}_{ij}) angle$	$\langle \mathscr{P}(1/r_{ij}^3) angle$	$E_{ m tot}$
-	⁹ Be	15500 16400 17000		-14.330 575 490 3 -14.330 575 988 0 -14.330 576 136 9 -14.330 576 79(8)	-268.220 833 -268.220 546 -268.220 503	-0.93445269 -0.93445125 -0.93444997	8.773 710 101 8.773 713 099 8.773 713 972	0.263 338 312 0.263 338 531 0.263 338 625	-1.271 53 -1.266 99 -1.265 58	-14.332549183 -14.332549665 -14.332549811 -14.332549811
$d_1 6$	°Be	$16\ 400 \\ 17\ 000 \\ \infty \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 16\ 400 \\ 10\ 40\ 400 \\ 10\ 40\ 400 \\ 10\ 40\ 40\ 400 \\ 10\ 40\ 40\ 40\ 40\ 40\ 40\ 40\ 40\ 40\ 4$	27 27	-14.330 575 975 973 2 -14.331 476 1248 -14.331 476 29(8) -14.331 475 953 7	-268.286 721	-0.9344530 -0.90805838 -0.9080607	8.775 331 042	0.263 382 359	-1.266 01	-14.333 449 712 -14.333 449 9(7)
10 ¹ S	⁹ Be ∞Be	15 000 16 000 17 000 8 00 17 000 8 00		$\begin{array}{c} -14.329\ 610\ 7179\\ -14.329\ 613\ 2641\\ -14.329\ 614\ 3144\\ -14.329\ 616\ 5(11)\\ -14.329\ 616\ 5(11)\\ -14.330\ 514\ 3414\\ -14.330\ 516\ 6(11)\end{array}$	-268.246 720 -268.246 831 -268.246 463 -268.312 694	-0.935 837 94 -0.935 827 86 -0.935 818 78 -0.909 422 21	8.774 463 692 8.774 482 339 8.774 494 082 8.776 111 519	0.263 372 106 0.263 373 330 0.263 374 247 0.263 417 990	-1.294 41 -1.286 64 -1.278 20 -1.278 64	$\begin{array}{c} -14.331584771\\ -14.331587302\\ -14.331588323\\ -14.331588323\\ -14.331591(14)\\ -14.332488262\\ -14.332490(14)\end{array}$
$10^{1}P$	⁹ Be ∞Be	15 500 16 400 17 000 8 16 400 17 000 8 8 16 400 17 000 16 400	27	$\begin{array}{c} -14.329\ 252\ 437\ 2\\ -14.329\ 255\ 100\ 6\\ -14.329\ 255\ 839\ 5\\ -14.329\ 255\ 4(3)\\ -14.329\ 255\ 009\ 9\\ -14.330\ 155\ 775\ 7\\ -14.330\ 156\ 3(3)\\ -14.330\ 156\ 3(3)\\ -14.330\ 154\ 912\ 7\end{array}$	-268.231 374 -268.230 280 -268.230 087 -268.230 087 -268.296 311	-0.934 976 66 -0.934 967 09 -0.934 967 09 -0.934 974 5 -0.908 572 88 -0.908 577 6	8.773 943 600 8.773 960 301 8.773 964 094 8.775 581 319	0.263 347 709 0.263 348 977 0.263 349 217 0.263 392 953	-1.295 66 -1.281 86 -1.279 28 -1.279 72	-14.331 226 367 -14.331 228 959 -14.331 229 684 -14.331 230 5(40) -14.332 129 533 -14.332 130 3(40)
11 ¹ S	⁹ Be ∞Be	15 000 16 000 17 000 8 00 17 000 8 00		-14.328 536 040 2 -14.328 547 329 0 -14.328 549 788 5 -14.328 556 5 (34) -14.329 449 730 7 -14.329 456 5 (34)	-268.250 503 -268.251 558 -268.250 488 -268.316 720	-0.935 922 20 -0.935 940 51 -0.935 930 94 -0.909 530 06	8.774 378 167 8.774 457 465 8.774 469 172 8.776 086 711	0.263 364 456 0.263 368 146 0.263 369 954 0.263 413 679	-1.334 33 -1.321 39 -1.311 73 -1.312 17	$\begin{array}{c} -14.330\ 510\ 390\\ -14.330\ 521\ 634\\ -14.330\ 524\ 007\\ -14.330\ 530\ 4(32)\\ -14.331\ 423\ 881\\ -14.331\ 423\ 881\\ -14.331\ 430\ 2(32)\end{array}$
11 ¹ <i>P</i>	⁹ Be ∞Be	15 000 16 000 17 000 8 16 400 17 000 8 16 400 16 400	27	$\begin{array}{c} -14.328\ 274\ 730\ 5\\ -14.328\ 276\ 608\ 0\\ -14.328\ 287\ 600\ 0\\ -14.328\ 287\ 870\ 0\\ -14.328\ 282\ 542\ 3\\ -14.329\ 187\ 765\ 9\\ -14.329\ 187\ 765\ 9\\ -14.329\ 187\ 241\ 1\\ -14.329\ 185\ 241\ 1\end{array}$	-268.236 832 -268.236 811 -268.236 605 -268.302 834	$\begin{array}{r} -0.93534441\\ -0.93534126\\ -0.93532084\\ -0.9353442\\ -0.90892279\\ -0.9089403\end{array}$	8.774 047 267 8.774 054 107 8.774 118 432 8.775 735 832	0.263 348 909 0.263 349 863 0.263 354 974 0.263 398 707	-1.320 58 -1.318 40 -1.295 65 -1.296 08	-14.330 248 804 -14.330 250 672 -14.330 261 848 -14.330 265 9(20) -14.331 161 656 -14.331 164 7(20)

TABLE 4. Transition energies, ΔE_{if} (in cm⁻¹). 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, $\Delta E_{if}^{\text{Exp}}$, have been taken from NIST Atomic Spectra Database (ver. 5.8).¹⁰¹ It should be noted that the experimental energy levels for $n^1P(n = 7-11)$ states in NIST ASD were determined by extrapolation of values with lower *n* using a quantum-defect expansion formula along the Rydberg series

Transition	$\Delta E_{if}(^{\infty}\mathrm{Be})$	ΔE_{if} (⁹ Be)	$\Delta E^{ m Exp}_{if}$
$2^{1}S \rightarrow 2^{1}P$	42 568.372(9)	42 565.443(9)	42 565.4502(10)
Ref. 4		42 565.441(11)	
$2^{1}S \rightarrow 3^{1}P$	60 191.905(7)	$60\ 187.444(7)$	60 187.443(21)
$2 {}^{1}S \rightarrow 4 {}^{1}P$	67 039.288(6)	67 034.814(6)	67 034.80(3)
$2 {}^{1}S \rightarrow 5 {}^{1}P$	70 125.089(6)	70 120.578(6)	70 120.59(3)
$2 {}^{1}S \rightarrow 6 {}^{1}P$	71 750.342(6)	71 745.796(6)	71 746.17(6)
$2 {}^{1}S \rightarrow 7 {}^{1}P$	72 705.938(11)	72 701.365(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)	73 719.51(2)	73 709.4(5)
$2 {}^{1}S \rightarrow 10 {}^{1}P$	74 013.86(8)	74 009.24(8)	74 009.2(5)
$2 {}^{1}S \rightarrow 11 {}^{1}P$	74 226.3(2)	74 221.7(2)	74 221.1(5)
$\frac{1}{2 P \rightarrow 3 S}$	12 112.435(4)	12 111.906(4)	12 111.898(21)
$2 P \rightarrow 4 S$	$22\ 681.144(4)$	$22\ 680.000(4)$	22 679.986(21)
$2^{1}P \rightarrow 5^{1}S$	26758.283(4)	26756.894(4)	26756.84(7)
$2 {}^{1}P \rightarrow 6 {}^{1}S$	28757.323(4)	28755.812(4)	28 755.79(8)
$2 {}^{1}P \rightarrow 7 {}^{1}S$	29 884.811(5)	29 883.232(5)	29 882.92(18)
$2 P \rightarrow 8 S$	30 582.82(3)	30 581.19(3)	30 581.21(19)
$2^{1}P \rightarrow 9^{1}S$	31 044.89(2)	31 043.24(2)	31 043.1(3)
$2 P \rightarrow 10 S$	31 366.767	31 365.09(11)	31 365.0(3)
$2 {}^{1}P \rightarrow 11 {}^{1}S$	31 600.4(3)	31 598.7(3)	31 598.0(3)
$\overline{3^{1}S \rightarrow 3^{1}P}$	5 511.098(3)	5 510.095(3)	5 510.094(30)
$3^{1}S \rightarrow 4^{1}P$	12358.480(1)	$12\ 357.465(1)$	12357.45(4)
$3^{1}S \rightarrow 5^{1}P$	15444.282(2)	15 443.230(2)	15443.24(4)
$3^{1}S \rightarrow 6^{1}P$	17 069.534(3)	17 068.447(3)	17068.82(6)
$3 {}^{1}S \rightarrow 7 {}^{1}P$	$18\ 025.131(10)$	18024.016(10)	18024.4(5)
$3^{1}S \rightarrow 8^{1}P$	18 633.09(3)	18 631.96(3)	18632.3(5)
$3^{1}S \rightarrow 9^{1}P$	19 043.31(2)	19 042.16(2)	19 032.0(5)
$3^{1}S \rightarrow 10^{1}P$	19 333.05(8)	19 331.89(8)	19 331.8(5)
$3^{1}S \rightarrow 11^{1}P$	19 545.5(2)	19 544.3(2)	19 543.7(5)
$3^{1}P \rightarrow 4^{1}S$	5 057.611(2)	5 057.998(2)	5 057.993(30)
$3^{1}P \rightarrow 5^{1}S$	9 134.750(2)	9 134.893(2)	9 134.856(73)
$3 P \rightarrow 6 S$	11 133.790(2)	11 133.811(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)	13421.24(2)	13 421.1(3)
$3 {}^{1}P \rightarrow 10 {}^{1}S$	13 743.22(11)	13 743.09(11)	13 743.0(3)
$3^{1}P \rightarrow 11^{1}S$	13 976.8(3)	13 976.7(3)	13 976.0(3)
$4 {}^{1}S \rightarrow 4 {}^{1}P$	1 789.771 6(10)	1 789.371 4(10)	1 789.36(37)
$4^{1}S \rightarrow 5^{1}P$	4875.573(1)	4 875.136(1)	4 875.15(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)
$4^{1}S \rightarrow 8^{1}P$	8 064.38(3)	8 063.86(3)	8 064.2(5)
$4^{1}S \rightarrow 9^{1}P$	8474.60(2)	8 474.06(2)	8 463.9(5)
$4^{1}S \rightarrow 10^{1}P$	8 764.35(8)	8 763.80(8)	8 763.7(5)
$4 {}^{1}S \rightarrow 11 {}^{1}P$	8 976.8(2)	8 976.2(2)	8 975.6(5)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Transition	$\Delta E_{if}(^{\infty}\mathrm{Be})$	$\Delta E_{if}({}^{9}\mathrm{Be})$	$\Delta E_{if}^{\mathrm{Exp}}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\overline{4^{1}P \rightarrow 5^{1}S}$	2 287.3679(9)	2 287.5231(9)	2 287.50(76)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$4 {}^{1}P \rightarrow 6 {}^{1}S$	4 286.4074(10)	4 286.4411(10)	4 286.45(85)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$4 {}^{1}P \rightarrow 7 {}^{1}S$	5 413.896(3)	5 413.861(3)	5 413.58(18)
$\begin{array}{cccccc} 4^1P \to 9^1S & 673.87(2) & 673.87(2) & 6573.87(3) \\ 4^1P \to 10^1S & 6895.84(11) & 6895.72(11) & 6895.73(3) \\ 4^1P \to 11^1S & 7129.4(3) & 7129.3(3) & 7128.7(3) \\ 5^1S \to 5^1P & 798.4338(9) & 798.2415(9) & 798.29(76) \\ 5^1S \to 6^1P & 2.423.686(2) & 2.423.459(2) & 2.423.87(92) \\ 5^1S \to 7^1P & 3.379.283(9) & 3.379.028(9) & 3.379.05(5) \\ 5^1S \to 9^1P & 4.397.46(2) & 4.397.17(2) & 4.387.1(5) \\ 5^1S \to 10^1P & 4.687.21(8) & 4.668.90(8) & 4.668.9(5) \\ 5^1S \to 10^1P & 4.687.21(8) & 4.668.90(8) & 4.668.9(5) \\ 5^1S \to 11^1P & 4.899.630(2) & 4.899.3(2) & 4.898.8(5) \\ \overline{5^1P \to 6^1S} & 1.200.6057(5) & 1.200.6764(5) & 1.200.667(4) \\ 5^1P \to 7^1S & 2.328.094(2) & 2.328.096(2) & 2.327.79(18) \\ 5^1P \to 1^1S & 3.488.17(2) & 3.488.10(2) & 3.488.01(3) \\ 5^1P \to 10^1S & 3.488.17(2) & 3.488.10(2) & 3.488.01(3) \\ 5^1P \to 10^1S & 3.488.17(2) & 3.488.10(2) & 3.488.01(3) \\ 5^1P \to 11^1S & 4.043.6(3) & 4.043.5(3) & 4.042.91(3) \\ 6^1S \to 6^1P & 1.380.243(9) & 1.380.110(9) & 1.380.5(5) \\ 6^1S \to 7^1P & 1.380.243(9) & 1.380.110(9) & 1.380.5(5) \\ 6^1S \to 9^1P & 2.398.42(2) & 2.398.25(2) & 2.388.1(5) \\ 6^1S \to 10^1P & 2.688.17(8) & 2.687.99(8) & 2.687.95(8) \\ 6^1S \to 10^1P & 2.688.17(8) & 2.687.99(8) & 2.687.95(5) \\ 6^1S \to 11^1P & 2.900.6(2) & 2.900.4(2) & 1.400.5(20) \\ 6^1P \to 8^1S & 1.400.85(2) & 1.400.84(2) & 1.400.5(20) \\ 6^1P \to 8^1S & 1.400.85(2) & 1.400.84(2) & 1.400.5(20) \\ 6^1P \to 9^1S & 1.862.92(2) & 1.862.88(2) & 1.862.43(3) \\ 6^1P \to 11^1S & 2.184.73(11) & 2.184.73(11) & 2.184.3(3) \\ 7^1S \to 7^1P & 2.52.755(6) & 2.52.691(6) & 2.53.4(5) \\ 7^1S \to 9^1P & 1.270.33(2) & 1.270.83(2) & 1.261.0(5) \\ 7^1S \to 9^1P & 1.270.32(2) & 1.773.0(2) & 1.772.7(5) \\ 7^1P \to 8^1S & 1.400.85(2) & 1.400.84(2) & 1.400.5(20) \\ 6^1P \to 11^1S & 2.418.4(3) & 2.418.3(3) & 2.417.3(3) \\ 7^1S \to 7^1P & 1.520.755(6) & 2.52.691(6) & 2.53.4(5) \\ 7^1S \to 10^1P & 1.560.68(8) & 1.560.57(8) & 1.560.8(5) \\ 7^1S \to 10^1P & 1.560.68(8) & 1.560.57(8) & 1.560.8(5) \\ 7^1S \to 10^1P & 1.560.68(8) & 1.560.57(8) & 1.560.8(5) \\ 7^1P \to 11^1S & 1.462.8(3) & 1.462.8(3) & 1.461.7(6) \\ 7^1P \to 11^1S & 1.46$	$4 {}^{1}P \rightarrow 8 {}^{1}S$	6 111.90(3)	6 111.82(3)	6 111.87(19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$4 {}^{1}P \rightarrow 9 {}^{1}S$	6 573.97(2)	6 573.87(2)	6 573.8(3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$4 {}^{1}P \rightarrow 10 {}^{1}S$	6 895.84(11)	6 895.72(11)	6 895.7(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$4 {}^{1}P \rightarrow 11 {}^{1}S$	7 129.4(3)	7 129.3(3)	7 128.7(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5^{1}S \rightarrow 5^{1}P$	798.4338(9)	798.2415(9)	798.29(76)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5^{1}S \rightarrow 6^{1}P$	2423.686(2)	2 423.459(2)	2 423.87(92)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5^{1}S \rightarrow 7^{1}P$	3 379.283(9)	3 379.028(9)	3 379.5(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5^{1}S \rightarrow 8^{1}P$	3 987.24(3)	3 986.97(3)	3987.4(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5^{1}S \rightarrow 9^{1}P$	4 397.46(2)	4 397.17(2)	4 387.1(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5^{1}S \rightarrow 10^{1}P$	4 687.21(8)	4 686.90(8)	4686.9(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 {}^{1}S \rightarrow 11 {}^{1}P$	4 899.630(2)	4 899.3(2)	4 898.8(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\overline{5^{1}P \to 6^{1}S}$	1 200.6057(5)	1 200.6764(5)	1 200.66(76)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 {}^{1}P \rightarrow 7 {}^{1}S$	2328.094(2)	2 328.096(2)	2 327.79(18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 {}^{1}P \rightarrow 8 {}^{1}S$	3 026.10(3)	3 026.06(3)	3026.0(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 {}^{1}P \rightarrow 9 {}^{1}S$	3 488.17(2)	3 488.10(2)	3 488.01(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 {}^{1}P \rightarrow 10 {}^{1}S$	3 810.04(11)	3 809.95(11)	3 809.91(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 {}^{1}P \rightarrow 11 {}^{1}S$	4 043.6(3)	4 043.5(3)	4 042.91(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\overline{6^1 S \rightarrow 6^1 P}$	424.647(2)	424.541(2)	424.92(10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6 {}^{1}S \rightarrow 7 {}^{1}P$	1 380.243(9)	1 380.110(9)	1 380.5(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6^{1}S \rightarrow 8^{1}P$	1 988.20(3)	1 988.05(3)	1988.4(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6^{1}S \rightarrow 9^{1}P$	2 398.42(2)	2 398.25(2)	2 388.1(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6^{1}S \rightarrow 10^{1}P$	2 688.17(8)	2 687.99(8)	2 687.9(5)
$6^{-1}P \rightarrow 7^{-1}S$ 702.8414(10)702.8786(10)702.21(19) $6^{-1}P \rightarrow 8^{-1}S$ 1 400.85(2)1 400.84(2)1 400.5(20) $6^{-1}P \rightarrow 9^{-1}S$ 1 862.92(2)1 862.88(2)1 862.4(3) $6^{-1}P \rightarrow 10^{-1}S$ 2 184.79(11)2 184.73(11)2 184.3(3) $6^{-1}P \rightarrow 11^{-1}S$ 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) $7^{-1}S \rightarrow 9^{-1}P$ 1 270.93(2)1 270.83(2)1 261.0(5) $7^{-1}S \rightarrow 10^{-1}P$ 1 560.68(8)1 560.57(8)1 560.8(5) $7^{-1}S \rightarrow 10^{-1}P$ 1 560.68(8)1 560.57(8)1 560.8(5) $7^{-1}S \rightarrow 11^{-1}P$ 1 773.1(2)1 773.0(2)1 772.7(5) $7^{-1}P \rightarrow 9^{-1}S$ 907.32(2)907.31(2)906.8(6) $7^{-1}P \rightarrow 11^{-1}S$ 1 229.19(11)1 229.16(11)1 228.7(6) $8^{-1}S \rightarrow 9^{-1}P$ 572.93(2)572.87(2)562.7(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) $8^{-1}S \rightarrow 10^{-1}P$ 862.67(8)862.61(8)862.5(5) $8^{-1}P \rightarrow 9^{-1}S$ 299.36(2)299.37(2)298.9(6) $8^{-1}P \rightarrow 9^{-1}S$ 299.36(2)299.37(2)298.9(6) $8^{-1}P \rightarrow 10^{-1}S$ 621.23(11)621.22(11)620.8(6) $8^{-1}P \rightarrow 10^{-1}S$ 621.23(11)621.22(11)620.8(6) $8^{-1}P \rightarrow 10^{-1}S$ 621.23(11)621.22(11) </td <td>$6^{1}S \rightarrow 11^{1}P$</td> <td>2 900.6(2)</td> <td>2 900.4(2)</td> <td>2 899.8(5)</td>	$6^{1}S \rightarrow 11^{1}P$	2 900.6(2)	2 900.4(2)	2 899.8(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6^{1}P \rightarrow 7^{1}S$	702.8414(10)	702.8786(10)	702.21(19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6 {}^{1}P \rightarrow 8 {}^{1}S$	1400.85(2)	1400.84(2)	1400.5(20)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6^{1}P \rightarrow 9^{1}S$	1862.92(2)	1862.88(2)	1862.4(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$6^{1}P \rightarrow 10^{1}S$	2 184.79(11)	2 184.73(11)	2 184.3(3)
$7^{1}S \rightarrow 7^{1}P$ $252.755(6)$ $252.691(6)$ $253.4(5)$ $7^{1}S \rightarrow 8^{1}P$ $860.72(3)$ $860.63(3)$ $861.3(5)$ $7^{1}S \rightarrow 9^{1}P$ $1270.93(2)$ $1270.83(2)$ $1261.0(5)$ $7^{1}S \rightarrow 10^{1}P$ $1560.68(8)$ $1560.57(8)$ $1560.8(5)$ $7^{1}S \rightarrow 11^{1}P$ $1773.1(2)$ $1773.0(2)$ $1772.7(5)$ $7^{1}P \rightarrow 8^{1}S$ $445.25(2)$ $445.27(2)$ $444.87(5)$ $7^{1}P \rightarrow 9^{1}S$ $907.32(2)$ $907.31(2)$ $906.8(6)$ $7^{1}P \rightarrow 10^{1}S$ $1229.19(11)$ $1229.16(11)$ $1228.7(6)$ $7^{1}P \rightarrow 11^{1}S$ $1462.8(3)$ $1462.8(3)$ $1461.7(6)$ $8^{1}S \rightarrow 8^{1}P$ $162.711(6)$ $162.669(6)$ $163.0(5)$ $8^{1}S \rightarrow 10^{1}P$ $862.67(8)$ $862.61(8)$ $862.5(5)$ $8^{1}S \rightarrow 10^{1}P$ $1075.1(2)$ $1075.0(2)$ $1074.4(5)$ $8^{1}P \rightarrow 10^{1}S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8^{1}P \rightarrow 10^{1}S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8^{1}P \rightarrow 11^{1}S$ $854.8(3)$ $854.8(3)$ $854.8(3)$	$6 {}^{1}P \rightarrow 11 {}^{1}S$	2 418.4(3)	2 418.3(3)	2 417.3(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$7^{1}S \rightarrow 7^{1}P$	252.755(6)	252.691(6)	253.4(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$7 {}^{1}S \rightarrow 8 {}^{1}P$	860.72(3)	860.63(3)	861.3(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$7 {}^{1}S \rightarrow 9 {}^{1}P$	1270.93(2)	1270.83(2)	1261.0(5)
$7 {}^1S \rightarrow 11 {}^1P$ $1773.1(2)$ $1773.0(2)$ $1772.7(5)$ $7 {}^1P \rightarrow 8 {}^1S$ $445.25(2)$ $445.27(2)$ $444.87(5)$ $7 {}^1P \rightarrow 9 {}^1S$ $907.32(2)$ $907.31(2)$ $906.8(6)$ $7 {}^1P \rightarrow 10 {}^1S$ $1229.19(11)$ $1229.16(11)$ $1228.7(6)$ $7 {}^1P \rightarrow 11 {}^1S$ $1462.8(3)$ $1462.8(3)$ $1461.7(6)$ $8 {}^1S \rightarrow 8 {}^1P$ $162.711(6)$ $162.669(6)$ $163.0(5)$ $8 {}^1S \rightarrow 9 {}^1P$ $572.93(2)$ $572.87(2)$ $562.7(5)$ $8 {}^1S \rightarrow 10 {}^1P$ $862.67(8)$ $862.61(8)$ $862.5(5)$ $8 {}^1S \rightarrow 11 {}^1P$ $1075.1(2)$ $1075.0(2)$ $1074.4(5)$ $8 {}^1P \rightarrow 9 {}^1S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 {}^1P \rightarrow 10 {}^1S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 {}^1P \rightarrow 11 {}^1S$ $854.8(3)$ $854.8(3)$ $854.8(3)$	$7 {}^{1}S \rightarrow 10 {}^{1}P$	1560.68(8)	1 560.57(8)	1560.8(5)
$7 \ ^1P \rightarrow 8 \ ^1S$ $445.25(2)$ $445.27(2)$ $444.87(5)$ $7 \ ^1P \rightarrow 9 \ ^1S$ $907.32(2)$ $907.31(2)$ $906.8(6)$ $7 \ ^1P \rightarrow 10 \ ^1S$ $1 \ 229.19(11)$ $1 \ 229.16(11)$ $1 \ 228.7(6)$ $7 \ ^1P \rightarrow 11 \ ^1S$ $1 \ 462.8(3)$ $1 \ 462.8(3)$ $1 \ 461.7(6)$ $8 \ ^1S \rightarrow 8 \ ^1P$ $162.711(6)$ $162.669(6)$ $163.0(5)$ $8 \ ^1S \rightarrow 9 \ ^1P$ $572.93(2)$ $572.87(2)$ $562.7(5)$ $8 \ ^1S \rightarrow 10 \ ^1P$ $862.67(8)$ $862.61(8)$ $862.5(5)$ $8 \ ^1S \rightarrow 11 \ ^1P$ $1 \ 075.1(2)$ $1 \ 075.0(2)$ $1 \ 074.4(5)$ $8 \ ^1P \rightarrow 9 \ ^1S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 \ ^1P \rightarrow 10 \ ^1S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 \ ^1P \rightarrow 11 \ ^1S$ $854.8(3)$ $854.8(3)$ $854.8(3)$	$7 {}^{1}S \rightarrow 11 {}^{1}P$	1 773.1(2)	1 773.0(2)	1 772.7(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$7^{1}P \rightarrow 8^{1}S$	445.25(2)	445.27(2)	444.87(5)
$7 ^1P \rightarrow 10 ^1S$ $1 229.19(11)$ $1 229.16(11)$ $1 228.7(6)$ $7 ^1P \rightarrow 11 ^1S$ $1 462.8(3)$ $1 462.8(3)$ $1 461.7(6)$ $8 ^1S \rightarrow 8 ^1P$ $162.711(6)$ $162.669(6)$ $163.0(5)$ $8 ^1S \rightarrow 9 ^1P$ $572.93(2)$ $572.87(2)$ $562.7(5)$ $8 ^1S \rightarrow 10 ^1P$ $862.67(8)$ $862.61(8)$ $862.5(5)$ $8 ^1S \rightarrow 11 ^1P$ $1 075.1(2)$ $1 075.0(2)$ $1 074.4(5)$ $8 ^1P \rightarrow 9 ^1S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 ^1P \rightarrow 10 ^1S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 ^1P \rightarrow 11 ^1S$ $854.8(3)$ $854.8(3)$ $854.8(3)$	$7 {}^{1}P \rightarrow 9 {}^{1}S$	907.32(2)	907.31(2)	906.8(6)
$7 \ ^1P \rightarrow 11 \ ^1S$ $1 \ 462.8(3)$ $1 \ 462.8(3)$ $1 \ 461.7(6)$ $8 \ ^1S \rightarrow 8 \ ^1P$ $162.711(6)$ $162.669(6)$ $163.0(5)$ $8 \ ^1S \rightarrow 9 \ ^1P$ $572.93(2)$ $572.87(2)$ $562.7(5)$ $8 \ ^1S \rightarrow 10 \ ^1P$ $862.67(8)$ $862.61(8)$ $862.5(5)$ $8 \ ^1S \rightarrow 11 \ ^1P$ $1 \ 075.1(2)$ $1 \ 075.0(2)$ $1 \ 074.4(5)$ $8 \ ^1P \rightarrow 9 \ ^1S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 \ ^1P \rightarrow 10 \ ^1S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 \ ^1P \rightarrow 11 \ ^1S$ $854.8(3)$ $854.8(3)$ $854.8(3)$	$7 {}^{1}P \rightarrow 10 {}^{1}S$	1 229.19(11)	1 229.16(11)	1228.7(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) $8 {}^{1}P \rightarrow 10 {}^{1}S$ 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)	$7 {}^{1}P \rightarrow 11 {}^{1}S$	1 462.8(3)	1 462.8(3)	1 461.7(6)
$8 {}^{1}S \rightarrow 9 {}^{1}P$ 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) $8 {}^{1}S \rightarrow 11 {}^{1}P$ 1 075.1(2)1 075.0(2)1 074.4(5) $8 {}^{1}P \rightarrow 9 {}^{1}S$ 299.36(2)299.37(2)298.9(6) $8 {}^{1}P \rightarrow 10 {}^{1}S$ 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)	$\overline{8 {}^{1}S \rightarrow 8 {}^{1}P}$	162.711(6)	162.669(6)	163.0(5)
$8 {}^{1}S \rightarrow 10 {}^{1}P$ $862.67(8)$ $862.61(8)$ $862.5(5)$ $8 {}^{1}S \rightarrow 11 {}^{1}P$ $1 075.1(2)$ $1 075.0(2)$ $1 074.4(5)$ $8 {}^{1}P \rightarrow 9 {}^{1}S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 {}^{1}P \rightarrow 10 {}^{1}S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 {}^{1}P \rightarrow 11 {}^{1}S$ $854.8(3)$ $854.8(3)$ $853.8(6)$	$8 {}^{1}S \rightarrow 9 {}^{1}P$	572.93(2)	572.87(2)	562.7(5)
$8 {}^{1}S \rightarrow 11 {}^{1}P$ $1 075.1(2)$ $1 075.0(2)$ $1 074.4(5)$ $8 {}^{1}P \rightarrow 9 {}^{1}S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 {}^{1}P \rightarrow 10 {}^{1}S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 {}^{1}P \rightarrow 11 {}^{1}S$ $854.8(3)$ $854.8(3)$ $853.8(6)$	$8 {}^{1}S \rightarrow 10 {}^{1}P$	862.67(8)	862.61(8)	862.5(5)
$8 \ ^1P \rightarrow 9 \ ^1S$ $299.36(2)$ $299.37(2)$ $298.9(6)$ $8 \ ^1P \rightarrow 10 \ ^1S$ $621.23(11)$ $621.22(11)$ $620.8(6)$ $8 \ ^1P \rightarrow 11 \ ^1S$ $854.8(3)$ $854.8(3)$ $853.8(6)$	$8 {}^{1}S \rightarrow 11 {}^{1}P$	1 075.1(2)	1 075.0(2)	1 074.4(5)
$\begin{array}{cccc} 8 \ ^{1}P \rightarrow 10 \ ^{1}S & 621.23(11) & 621.22(11) & 620.8(6) \\ 8 \ ^{1}P \rightarrow 11 \ ^{1}S & 854 \ 8(3) & 854 \ 8(3) & 853 \ 8(6) \end{array}$	$\overline{8 {}^{1}P \rightarrow 9 {}^{1}S}$	299.36(2)	299.37(2)	298.9(6)
$8^{1}P \rightarrow 11^{1}S$ $854.8(3)$ $854.8(3)$ $854.8(3)$	$8 {}^{1}P \rightarrow 10 {}^{1}S$	621.23(11)	621.22(11)	620.8(6)
000000000000000000000000000000000000000	$8 {}^{1}P \rightarrow 11 {}^{1}S$	854.8(3)	854.8(3)	853.8(6)

TABLE 4.	(Continued)
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TABLE 4. (Continued)

Transition	$\Delta E_{if}(^{\infty}\mathrm{Be})$	$\Delta E_{if}({}^{9}\mathrm{Be})$	$\Delta E_{if}^{\mathrm{Exp}}$	
$9^{1}S \rightarrow 9^{1}P$	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)	613.0(2)	612.5(6)	
$9^{1}P \rightarrow 10^{1}S$	211.01(10)	211.02(10)	221.1(6)	
$9 {}^{1}P \rightarrow 11 {}^{1}S$	444.62(2)	445.13(2)	454.1(6)	
$10^{1}S \rightarrow 10^{1}P$	78.73(3)	78.71(3)	78.7(6)	
$10 {}^{1}S \rightarrow 11 {}^{1}P$	291.2(2)	291.1(2)	290.6(6)	
$10 {}^{1}P \rightarrow 11 {}^{1}S$	154.9(2)	154.9(2)	154.3(6)	
$11 {}^{1}S \rightarrow 11 {}^{1}P$	57.6(2)	57.5(2)	57.6(6)	
-				

TABLE 5. The squares of the transition dipole moments, $|\mu_{if}|^2$, and oscillator strengths, f_{if} , between ¹S and ¹P states. For $|\mu_{if}|^2$, 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 $|\mu_{if}|^2$ and ΔE_{if} . Numbers in square brackets, [s], denote a multiplication factor 10^s

Transition	$ \mu_{if} ^2$ (^{∞} Be)	$ \mu_{if} ^2 (^9 \text{Be})$	f_{if} (^{∞} Be)	f_{if} (⁹ Be)	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{a}}$	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{b}}$	$f_{if} ({}^{\infty}\mathrm{Be})^{c}$
$\overline{2^{1}S \rightarrow 2^{1}P}$	1.063 146 385(10) [+1]	1.063 255 365(10) [+1]	1.374 689 2(3) [0]	1.374 400 8(3) [0]	1.375 [0]	1.38 [0]	1.380 [0]
$2^{1}S \rightarrow 3^{1}P$	4.703 28(2) [-2]	4.695 34(2) [-2]	8.599 31(4) [-3]	8.582 06(4) [-3]	9.01 [-3]	8.98 [-3]	8.985 [-3]
$2 {}^{1}S \rightarrow 4 {}^{1}P$	1.31961(4) [-3]	1.329 66(4) [-3]	2.687 20(9) [-4]	2.706 82(9) [-4]	2.30 [-4]	1.20 [-4]	
$2 {}^{1}S \rightarrow 5 {}^{1}P$	4.026 52(7) [-3]	4.038 60(7) [-3]	8.576 84(14) [-4]	8.599 94(14) [-4]	8.10 [-4]	6.90 [-4]	
$2^{1}S \rightarrow 6^{1}P$	3.622 30(13) [-3]	3.63070(13) [-3]	7.8947(3) [-4]	7.9105(3)[-4]	7.50 [-4]	6.80 [-4]	
$2 {}^{1}S \rightarrow 7 {}^{1}P$	2.760 62(14) [-3]	2.766 31(14) [-3]	6.0968(3)[-4]	6.107 5(3) [-4]	5.90 [-4]	5.40 [-4]	
$2^{1}S \rightarrow 9^{1}P$	1.524 52(2) [-3]	1.527 54(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]			
$2 {}^{1}S \rightarrow 11 {}^{1}P$	8.90(7) [-4]	8.92(7) [-4]	2.01(2) [-4]	2.01(2) [-4]			
$\overline{2^{1}P \rightarrow 3^{1}S}$	9.613 578 7(15) [0]	9.613 186 1(15) [0]	1.1790161(5)[-1]	1.178 629 3(5) [-1]	1.18 [-1]	1.15 [-1]	1.147 [-1]
$2 {}^{1}P \rightarrow 4 {}^{1}S$	4.280 48(6) [-1]	4.280 54(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]	1.972 9(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]	1.278 05(3) [-3]	1.23 [-3]	1.18 [-3]	
$2 {}^{1}P \rightarrow 8 {}^{1}S$	2.94373(5) [-2]	2.945 90(5) [-2]	9.115 45(15) [-4]	9.119 48(15) [-4]	9.08 [-4]	8.11 [-4]	
$2 {}^{1}P \rightarrow 9 {}^{1}S$	2.19374(2) [-2]	2.196 04(2) [-2]	6.89571(8) [-4]	6.900 87(8) [-4]	6.94 [-4]	5.92 [-4]	
$2 {}^{1}P \rightarrow 10 {}^{1}S$	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]			
$\overline{3^{1}S \rightarrow 3^{1}P}$	5.713 342 8(3) [+1]	5.713 911 1(3) [+1]	9.564 292(5) [-1]	9.561 174(5) [-1]	9.58 [-1]	9.57 [-1]	9.465 [-1]
$3^{1}S \rightarrow 4^{1}P$	2.762 51(5) [-1]	2.769 26(5) [-1]	1.037 04(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]	3.157 18(2) [-1]	1.479 26(8) [-2]	1.480 66(8) [-2]	1.45 [-2]	1.45 [-2]	
$3^{1}S \rightarrow 6^{1}P$	2.103 53(5) [-1]	2.10571(5) [-1]	1.090 67(2) [-2]	1.091 47(2) [-2]	1.07 [-2]	1.08 [-2]	
$3^{1}S \rightarrow 7^{1}P$	1.389 96(2) [-1]	1.391 27(2) [-1]	7.61034(14) [-3]	7.615 22(14) [-3]	7.51 [-3]	7.50 [-3]	
$3^{1}S \rightarrow 8^{1}P$	9.503 6(5) [-2]	9.5126(5)[-2]	5.3790(3)[-3]	5.382 4(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]	3.900 4(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]			
$3^{1}S \rightarrow 11^{1}P$	3.72(3) [-2]	3.72(3) [-2]	2.21(2) [-3]	2.21(2) [-3]			
$3^{1} \overline{P \rightarrow 4^{1} S}$	4.060 230(3) [+1]	4.059 474(3) [+1]	2.079214(2) [-1]	2.078 480(2) [-1]	2.09 [-1]	2.12 [-1]	
$3 {}^{1}P \rightarrow 5 {}^{1}S$	2.630 541(4) [0]	2.630732(4) [0]	2.433 016(3) [-2]	2.432 638(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]	8.581 3(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]	4.230 8(6) [-3]	4.23 [-3]	4.22 [-3]	

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TABLE 5. ((Continued)
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Transition	$ \mu_{if} ^2 (^{\infty} \mathrm{Be})$	$ \mu_{if} ^2 (^9 \text{Be})$	f_{if} (^{∞} Be)	f _{if} (⁹ Be)	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{a}}$	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{b}}$	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{c}}$
$3 {}^{1}P \rightarrow 8 {}^{1}S$ $3 {}^{1}P \rightarrow 9 {}^{1}S$ $3 {}^{1}P \rightarrow 10 {}^{1}S$ $3 {}^{1}P \rightarrow 11 {}^{1}S$	1.874 3(3) [-1] 1.161 85(10) [-1] 7.791(9) [-2] 5.53(2) [-2]	1.875 0(3) [-1] 1.162 45(10) [-1] 7.796(9) [-2] 5.54(2) [-2]	2.459 3(4) [-3] 1.578 89(13) [-3] 1.084(13) [-3] 7.83(3) [-4]	2.459 6(4) [-3] 1.579 30(13) [-3] 1.085(13) [-3] 7.83(3) [-4]	2.47 [-3] 1.60 [-3] 1.14 [-3]	2.44 [-3] 1.56 [-3]	
$ \frac{4 {}^{1}S \rightarrow 4 {}^{1}P}{4 {}^{1}S \rightarrow 5 {}^{1}P} \\ 4 {}^{1}S \rightarrow 5 {}^{1}P}{4 {}^{1}S \rightarrow 6 {}^{1}P} \\ 4 {}^{1}S \rightarrow 7 {}^{1}P \\ 4 {}^{1}S \rightarrow 8 {}^{1}P \\ 4 {}^{1}S \rightarrow 9 {}^{1}P \\ 4 {}^{1}S \rightarrow 10 {}^{1}P \\ 4 {}^{1}S \rightarrow 11 {}^{1}P $	$\begin{array}{c} 2.631\ 297\ 0(6)\ [+2]\\ 1.230\ 43(14)\ [-1]\\ 2.616\ 7(2)\ [-1]\\ 1.857\ 1(8)\ [-1]\\ 1.256\ 3(2)\ [-1]\\ 8.726(2)\ [-2]\\ 6.269(6)\ [-2]\\ 4.65(3)\ [-2] \end{array}$	$\begin{array}{c} 2.6317086(6)[+2]\\ 1.23764(14)[-1]\\ 2.6222(2)[-1]\\ 1.8600(8)[-1]\\ 1.2580(2)[-1]\\ 8.738(2)[-2]\\ 6.278(6)[-2]\\ 4.66(3)[-2] \end{array}$	$\begin{array}{c} 1.430\ 513\ 2(9)\ [0]\\ 1.822\ 24(20)\ [-3]\\ 5.167\ 1(4)\ [-3]\\ 4.206(2)\ [-3]\\ 3.077\ 4(5)\ [-3]\\ 2.246(5)\ [-3]\\ 1.669(2)\ [-3]\\ 1.27(9)\ [-3] \end{array}$	1.430 068 9(9) [0] 1.832 31(20) [-3] 5.176 4(4) [-3] 4.212(2) [-3] 3.080 8(5) [-3] 2.249(5) [-3] 1.671(2) [-3] 1.27(9) [-3]	1.43 [0] 1.59 [-3] 4.95 [-3] 4.08 [-3] 2.98 [-3] 2.16 [-3]	1.67 [-3] 5.10 [-3] 4.17 [-3] 2.71 [-3] 2.23 [-3]	
$\begin{array}{c} 4 {}^{1}P \rightarrow 5 {}^{1}S \\ 4 {}^{1}P \rightarrow 6 {}^{1}S \\ 4 {}^{1}P \rightarrow 7 {}^{1}S \\ 4 {}^{1}P \rightarrow 8 {}^{1}S \\ 4 {}^{1}P \rightarrow 9 {}^{1}S \\ 4 {}^{1}P \rightarrow 10 {}^{1}S \\ 4 {}^{1}P \rightarrow 11 {}^{1}S \end{array}$	$\begin{array}{l} 1.266\ 409(2)\ [+2]\\ 8.287\ 77(7)\ [0]\\ 2.312\ 0(5)\ [0]\\ 1.009\ 2(2)\ [0]\\ 5.459\ 4(6)\ [-1]\\ 3.348(3)\ [-1]\\ 2.232(8)\ [-1] \end{array}$	$\begin{array}{l} 1.266\ 156(2)\ [+2]\\ 8.288\ 28(7)\ [0]\\ 2.312\ 4(5)\ [0]\\ 1.009\ 5(2)\ [0]\\ 5.461\ 7(6)\ [-1]\\ 3.351(3)\ [-1]\\ 2.234(8)\ [-1] \end{array}$	$\begin{array}{l} 2.933\ 007(4)\ [-1]\\ 3.596\ 95(3)\ [-2]\\ 1.267\ 4(3)\ [-2]\\ 6.245\ 3(11)\ [-3]\\ 3.634\ 0(4)\ [-3]\\ 2.338(2)\ [-3]\\ 1.611(6)\ [-3] \end{array}$	$\begin{array}{l} 2.931\ 905(4)\ [-1]\\ 3.596\ 32(3)\ [-2]\\ 1.267\ 2(3)\ [-2]\\ 6.245\ 4(11)\ [-3]\\ 3.634\ 5(4)\ [-3]\\ 2.339(2)\ [-3]\\ 1.612(6)\ [-3] \end{array}$	2.95 [-1] 3.60 [-3] 1.27 [-2] 6.27 [-3] 3.69 [-3] 2.45 [-3]	3.61 [-3] 1.27 [-2] 6.25 [-3] 3.63 [-3]	
$\overline{\begin{array}{c}5 \\ 5 \\ 5 \\ 5 \\ 5 \\ 5 \\ 5 \\ 5 \\ 7 \\ 1P \\ 5 \\ 5 \\ 7 \\ 1P \\ 5 \\ 5 \\ 7 \\ 1P \\ 5 \\ 1S \\ 7 \\ 1P \\ 5 \\ 1S \\ 7 \\ 1P \\ 5 \\ 1S \\ 10 \\ 1P \\ 5 \\ 1S \\ 11 \\ 1P \end{array}}$	7.481 658(8) [+2] 8.401(5) [-2] 3.272(4) [-1] 2.420 7(9) [-1] 1.673(3) [-1] 1.179(2) [-1] 8.57(5) [-2]	$7.482926(8)\ [+2]\\8.496(5)\ [-2]\\3.281(4)\ [-1]\\2.4248(9)\ [-1]\\1.676(3)\ [-1]\\1.181(2)\ [-1]\\8.59(5)\ [-2]$	1.814 518(3) [0] 6.185(3) [-4] 3.359(4) [-3] 2.931 8(11) [-3] 2.235(4) [-3] 1.679(3) [-3] 1.28(7) [-3]	1.813 946(3) [0] 6.253(3) [-4] 3.367(4) [-3] 2.935 9(11) [-3] 2.237(4) [-3] 1.681(3) [-3] 1.28(7) [-3]	1.82 [0] 4.78 [-4] 3.16 [-3] 2.79 [-3] 2.10 [-3]	3.32 [-3] 2.59 [-3] 2.22 [-3]	
$ \frac{5^{1}P \to 6^{1}S}{5^{1}P \to 7^{1}S} \\ 5^{1}P \to 8^{1}S \\ 5^{1}P \to 9^{1}S \\ 5^{1}P \to 10^{1}S \\ 5^{1}P \to 11^{1}S $	3.157 64(2) [+2] 2.031 3(2) [+1] 5.498 6(8) [0] 2.350(2) [0] 1.257(3) [0] 7.66(3) [-1]	3.157 04(2) [+2] 2.031 5(2) [+1] 5.499 8(8) [0] 2.351(2) [0] 1.257(3) [0] 7.67(3) [-1]	3.838 54(3) [-1] 4.788 4(6) [-2] 1.684 8(3) [-2] 8.299(9) [-3] 4.848(12) [-3] 3.14(13) [-3]	3.837 10(3) [-1] 4.787 6(6) [-2] 1.684 7(3) [-2] 8.300(9) [-3] 4.849(12) [-3] 3.14(13) [-3]	3.86 [-1] 4.79 [-2] 1.69 [-2] 8.45 [-2] 5.10 [-2]	8.32 [-3]	
$6^{1}S \to 6^{1}P$ $6^{1}S \to 7^{1}P$ $6^{1}S \to 8^{1}P$ $6^{1}S \to 9^{1}P$ $6^{1}S \to 10^{1}P$ $6^{1}S \to 11^{1}P$	1.691 681(10) [+3] 4.85(2) [-2] 4.238(8) [-1] 3.257(13) [-1] 2.272(6) [-1] 1.606(4) [-1]	1.691 971(10) [+3] 4.96(2) [-2] 4.251(8) [-1] 3.261(13) [-1] 2.276(6) [-1] 1.608(4) [-1]	2.182 081(16) [0] 2.03(9) [-4] 2.560(5) [-3] 2.373(9) [-3] 1.855(5) [-3] 1.415(3) [-3]	2.181 379(16) [0] 2.08(9) [-4] 2.567(5) [-3] 2.375(9) [-3] 1.858(5) [-3] 1.417(3) [-3]	2.19 [0] 1.12 [-4] 2.30 [-3] 2.12 [-3]		
$6^{1}P \to 7^{1}S \\ 6^{1}P \to 8^{1}S \\ 6^{1}P \to 9^{1}S \\ 6^{1}P \to 10^{1}S \\ 6^{1}P \to 11^{1}S \\ 6^{1}P \to 11^{1}S \\ \hline$	6.706 9(4) [+2] 4.231(2) [+1] 1.119 4(14) [+1] 4.705(3) [0] 2.485(6) [0]	6.705 8(4) [+2] 4.231(2) [+1] 1.119 7(14) [+1] 4.708(3) [0] 2.487(6) [0]	4.772 9(3) [-1] 6.001(2) [-2] 2.111 4(26) [-2] 1.041(7) [-2] 6.084(16) [-3]	4.771 2(3) [-1] 6.000(2) [-2] 2.111 4(26) [-2] 1.041(7) [-2] 6.088(16) [-3]	4.79 [-1] 6.03 [-2] 2.15 [-2] 1.10 [-2]		
$7 {}^{1}S \rightarrow 7 {}^{1}P$ $7 {}^{1}S \rightarrow 8 {}^{1}P$ $7 {}^{1}S \rightarrow 9 {}^{1}P$	3.316 5(2) [+3] 1.307(7) [-2] 5.380(8) [-1]	3.317 0(2) [+3] 1.387(7) [-2] 5.384(8) [-1]	2.546 2(2) [0] 3.418(19) [-5] 2.077(3) [-3]	2.545 4(2) [0] 3.624(19) [-5] 2.078(3) [-3]	2.56 [0] 5.00 [-8] 1.64 [-3]	5.00 [-8]	

Transition	$ \mu_{if} ^2 (^{\infty} \text{Be})$	$ \mu_{if} ^2 (^9 \text{Be})$	f_{if} (^{∞} Be)	f _{if} (⁹ Be)	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{a}}$	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{b}}$	$f_{if} ({}^{\infty}\mathrm{Be})^{\mathrm{c}}$
$7^{1}S \rightarrow 10^{1}P$ $7^{1}S \rightarrow 11^{1}P$	4.31(3) [-1] 3.00(6) [-1]	4.30(3) [-1] 3.00(6) [-1]	2.04(1) [-3] 1.62(3) [-3]	2.04(1) [-3] 1.62(3) [-3]			
$\overline{7 {}^{1}P \rightarrow 8 {}^{1}S}$ $7 {}^{1}P \rightarrow 9 {}^{1}S$ $7 {}^{1}P \rightarrow 10 {}^{1}S$ $7 {}^{1}P \rightarrow 11 {}^{1}S$	1.269 9(3) [+3] 7.869(7) [+1] 2.045(5) [+1] 8.46(4) [0]	1.2697(3) [+3] 7.869(7) [+1] 2.046(5) [+1] 8.47(4) [0]	5.725 2(13) [-1] 7.229(6) [-2] 2.546(6) [-2] 1.25(5) [-2]	5.723 2(13) [-1] 7.228(6) [-2] 2.546(6) [-2] 1.25(5) [-2]	5.75 [-1] 7.33 [-2] 2.68 [-2]		
$ \frac{8 {}^{1}S \rightarrow 8 {}^{1}P}{8 {}^{1}S \rightarrow 9 {}^{1}P} \\ 8 {}^{1}S \rightarrow 10 {}^{1}P}{8 {}^{1}S \rightarrow 11 {}^{1}P} $	5.888 2(12) [+3] 1.6(4) [-3] 6.59(4) [-1] 5.42(14) [-1]	5.888 9(12) [+3] 1.3(4) [-3] 6.57(4) [-1] 5.41(14) [-1]	2.910 2(6) [0] 2.8(8) [-6] 1.73(1) [-3] 1.77(5) [-3]	2.909 1(6) [0] 2.3(8) [-6] 1.72(1) [-3] 1.76(5) [-3]	2.94 [0] 1.47 [-6]		
$ \frac{8 {}^{1}P \rightarrow 9 {}^{1}S}{8 {}^{1}P \rightarrow 10 {}^{1}S} \\ 8 {}^{1}P \rightarrow 11 {}^{1}S $	2.207 0(8) [+3] 1.349(7) [+2] 3.47(5) [+1]	2.206 5(8) [+3] 1.349(7) [+2] 3.47(5) [+1]	6.689 5(24) [-1] 8.49(4) [-2] 3.00(5) [-2]	6.686 9(24) [-1] 8.48(4) [-2] 3.00(5) [-2]	6.73 [-2] 8.82 [-2]		
$ \frac{9 {}^{1}S \rightarrow 9 {}^{1}P}{9 {}^{1}S \rightarrow 10 {}^{1}P} \\ 9 {}^{1}S \rightarrow 11 {}^{1}P $	9.7199(11) [+3] 5.(5) [-2] 8.(2) [-1]	9.7207(11)[+3] 5.(5)[-2] 8.(2)[-1]	3.273 0(4) [0] 6.(6) [-5] 1.(3) [-3]	3.271 6(4) [0] 6.(6) [-5] 1.(3) [-3]	3.34 [0]		
$9^{1}P \rightarrow 10^{1}S$ $9^{1}P \rightarrow 11^{1}S$	3.583(13) [+3] 2.19(6) [+2]	3.582(13) [+3] 2.19(6) [+2]	7.656(27) [-1] 9.84(26) [-2]	7.652(27) [-1] 9.85(26) [-2]	7.80 [-1]		
$\frac{10^{1}S \to 10^{1}P}{10^{1}S \to 11^{1}P}$	1.519(5) [+4] 1.(2) [-1]	1.519(5) [+4] 1.(2) [-1]	3.632(12) [0] 1.(2) [-4]	3.630(12) [0] 1.(2) [-4]			
$10^{1}P \rightarrow 11^{1}S$	5.50(7) [+3]	5.49(7) [+3]	8.62(11) [-1]	8.61(11) [-1]			
$11 {}^1S \rightarrow 11 {}^1P$	2.28(4) [+4]	2.28(4) [+4]	3.98(7) [0]	3.98(7) [0]			

TABLE 5. (Continued)

^aB-spline CI with semi-empirical core potential (BCICP) method.¹⁰²

^bMCHF method.¹¹

^cB-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 2¹S \rightarrow 2¹P 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 CI with semi-empirical core potential (BCICP), B-spline CI (BCIBP), and CI+ core polarization (CICP)

Experimental				
BF ¹⁰⁴	1.34(4)			
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 ($^{\infty}$ Be)	1.374 689 2(3)			
this work (⁹ Be)	1.374 400 8(3)			



FIG. 2. The density of the nucleus for some of the ¹S (left-column) and ¹P 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 ¹S (left-column) and ¹P 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 ⁹Be 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 ¹P, one finds that all experimental and the calculated results differ by about 10 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 ⁹Be and ^{∞}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., $n^1S \rightarrow n^1P$ transitions. However, the oscillator strength values are also quite sizable for the $n^1P \rightarrow (n + 1)^1S$ transitions. This indicates a possibility to use "cascade" excitations involving a sequence of the following transitions: $2 \, {}^1S \rightarrow 2 \, {}^1P$, $2 \, {}^1P \rightarrow 3 \, {}^1S$, $3 \, {}^1S \rightarrow 3 \, {}^1P$, $3 \, {}^1P \rightarrow 4 \, {}^1S$, 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 ${}^{9}Be$ and ${}^{\infty}Be$ 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 $n^1S \rightarrow n^1P$ and $n^{1}P \rightarrow (n+1)^{1}S$ transitions, one can envision preparing a beryllium atoms in a particular excited Rydberg ¹S or ¹P 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 ²S 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.

6. References

¹E. Träbert, P. Beiersdorfer, N. S. Brickhouse, and L. Golub, "High-resolution laboratory spectra of the λ 193 channel of the atmospheric imaging assembly instrument on board Solar Dynamics Observatory," Astrophys. J., Suppl. Ser. **215**, 6 (2014).

²E. Träbert, P. Beiersdorfer, N. S. Brickhouse, and L. Golub, "High-resolution laboratory spectra on the λ 131 channel of the AIA instrument on board the Solar Dynamics Observatory," Astrophys. J., Suppl. Ser. **211**, 14 (2014).

³Z.-C. Yan and G. W. F. Drake, "Eigenvalues and expectation values for the $1s^22s^2S$, $1s^22p^2P$, and $1s^23d^2D$ states of lithium," Phys. Rev. A **52**, 3711 (1995).

⁴M. Puchalski, K. Pachucki, and J. Komasa, "Isotope shift in a beryllium atom," Phys. Rev. A **89**, 012506 (2014).

⁵S. Nasiri, T. Shomenov, S. Bubin, and L. Adamowicz, "High-accuracy calculations of the lowest eleven Rydberg ²P states of Li atom," J. Phys. B: At., Mol. Opt. Phys. 54, 085003 (2021).

⁶I. Hornyák, S. Nasiri, S. Bubin, and L. Adamowicz, ^{«2}*S* Rydberg spectrum of the boron atom," Phys. Rev. A **104**, 032809 (2021).

⁷J. Fleming, A. Hibbert, and R. P. Stafford, "The 1909 Å intercombination line in C III," Phys. Scr. **49**, 316 (1994).

⁸J. Fleming, T. Brage, K. L. Bell, N. Vaeck, A. Hibbert, M. R. Godefroid, and C. Froese Fischer, "Systematic studies of N IV transitions of astrophysical importance," Astrophys. J. **455**, 758 (1995).

⁹J. Fleming, N. Vaeck, A. Hibbert, K. L. Bell, and M. R. Godefroid, "Oscillator strengths for the resonance line of ions in the beryllium isoelectronic sequence," Phys. Scr. **53**, 446 (1996).

¹⁰ A. Hibbert, "CIV3—A general program to calculate configuration interaction wave functions and electric-dipole oscillator strengths," Comput. Phys. Commun. 9, 141 (1975).

¹¹G. Tachiev and C. Froese Fischer, "Breit-Pauli energy levels, lifetimes, and transition data: Beryllium-like spectra," J. Phys. B: At., Mol. Opt. Phys. **32**, 5805 (1999).

¹² A. Ynnerman and C. Froese Fischer, "Multiconfigurational-Dirac-Fock calculation of the $2s^{21} S_0$ – $2s2p^3P_1$ spin-forbidden transition for the Be-like isoelectronic sequence," Phys. Rev. A **51**, 2020 (1995).

¹³E. A. Hylleraas, "Neue berechnung der energie des heliums im grundzustande, sowie des tiefsten terms von ortho-helium," Z. Phys. 54, 347 (1929).

 14 G. W. F. Drake, M. M. Cassar, and R. A. Nistor, "Ground-state energies for helium, H⁻ and Ps⁻," Phys. Rev. A **65**, 054501 (2002).

¹⁵C. Schwartz, "Experiment and theory in computations of the He atom ground state," Int. J. Mod. Phys. E 15, 877 (2006).

¹⁶C. Schwartz, "Further computations of the He atom ground state," arXiv:mathph/0605018 (2006).

¹⁷H. Nakashima and H. Nakatsuji, "Solving the electron-nuclear Schrödinger equation of helium atom and its isoelectronic ions with the free iterative-complement-interaction method," J. Chem. Phys. **128**, 154107 (2008).

¹⁸V. A. Yerokhin and K. Pachucki, "Theoretical energies of low-lying states of light helium-like ions," Phys. Rev. A 81, 022507 (2010).

¹⁹D. T. Aznabaev, A. K. Bekbaev, and V. I. Korobov, "Nonrelativistic energy levels of helium atoms," Phys. Rev. A 98, 012510 (2018).

²⁰J. S. Sims and S. A. Hagstrom, "Hylleraas-configuration-interaction study of the 2^2S ground state of neutral lithium and the first five excited ²S states," Phys. Rev. A **80**, 052507 (2009).

²¹K. Pachucki and A. M. Moro, "Nuclear polarizability of helium isotopes in atomic transitions," Phys. Rev. A **75**, 032521 (2007).

²²L. M. Wang, Z.-C. Yan, H. X. Qiao, and G. W. F. Drake, "Variational energies and the Fermi contact term for the low-lying states of lithium: Basis-set completeness," Phys. Rev. A 85, 052513 (2012).

²³ M. Puchalski, J. Komasa, and K. Pachucki, "Testing quantum electrodynamics in the lowest singlet states of the beryllium atom," Phys. Rev. A 87, 030502 (2013).

²⁴M. Stanke, J. Komasa, S. Bubin, and L. Adamowicz, "Five lowest ¹S states of the Be atom calculated with a finite-nuclear-mass approach and with relativisti1c and QED corrections," Phys. Rev. A **80**, 022514 (2009).

²⁵S. Bubin, J. Komasa, M. Stanke, and L. Adamowicz, "Isotope shifts of the $1s^22s^2({}^{1}S_0) \rightarrow 1 s^22p^2({}^{1}S_0)$ transition in the doubly ionized carbon ion C²⁺," Phys. Rev. A **81**, 052504 (2010).

²⁶I. Hornyák, L. Adamowicz, and S. Bubin, "Ground and excited ¹S states of the beryllium atom," Phys. Rev. A **100**, 032504 (2019). ²⁷ M. Stanke, S. Bubin, and L. Adamowicz, "Lowest ten ¹P Rydberg states of beryllium calculated with all-electron explicitly correlated Gaussian functions," J. Phys. B: At., Mol. Opt. Phys. 52, 155002 (2019).

²⁸ E. C. Cook, A. D. Vira, C. Patterson, E. Livernois, and W. D. Williams, "Testing quantum electrodynamics in the lowest singlet state of neutral beryllium-9," Phys. Rev. Lett. **121**, 053001 (2018).

²⁹W. R. Bozman, C. H. Corliss, W. F. Meggers, and R. E. Trees, "An intersystem transition in the first spectrum of beryllium," J. Res. Natl. Bur. Stand. 50, 131 (1953).

³⁰L. Johansson, "The spectrum of the neutral beryllium atom," Ark. Fys. 23, 119 (1963).

³¹D. R. Hartree and W. Hartree, "Self-consistent field, with exchange, for beryllium," Proc. R. Soc. London, Ser. A **150**, 9 (1935).

³²S. F. Boys, "Electronic wave functions. II. A calculation for the ground state of the beryllium atom," Proc. R. Soc. London, Ser. A 201, 125 (1950).

³³S. F. Boys, "Electronic wave functions IX. Calculations for the three lowest states of the beryllium atom," Proc. R. Soc. London, Ser. A 217, 136 (1953).

³⁴G. H. Brigman, R. P. Hurst, J. D. Gray, and F. A. Matsen, "Open configuration calculations for beryllium," J. Chem. Phys. 29, 251 (1958).

³⁵R. E. Watson, "Approximate wave functions for atomic Be," Phys. Rev. 119, 170 (1960).

³⁶A. W. Weiss, "Configuration interaction in simple atomic systems," Phys. Rev. 122, 1826 (1961).

³⁷H. P. Kelly, "Correlation effects in atoms," Phys. Rev. 131, 684 (1963).

³⁸L. Szasz and J. Byrne, "Atomic many-body problem. III. The calculation of hylleraas-type correlated wave functions for the beryllium atom," Phys. Rev. **158**, 34 (1967).

³⁹R. F. Gentner and E. A. Burke, "Calculation of the ¹S state of the beryllium atom in Hylleraas coordinates," Phys. Rev. **176**, 63 (1968).

⁴⁰C. F. Bunge, "Electronic wave functions for atoms. I. Ground state of Be," Phys. Rev. 168, 92 (1968).

⁴¹J. S. Sims and S. Hagstrom, "Combined configuration-interaction-hylleraastype wave-function study of the ground state of the beryllium atom," Phys. Rev. A 4, 908 (1971).

⁴²J. F. Perkins, "Hylleraas-type calculations of the Be ground state," Phys. Rev. A 8, 700 (1973).

 43 C. Froese Fischer and K. M. S. Saxena, "Correlation study of Be $1s^22s^2$ by a separated-pair numerical multiconfiguration Hartree-Fock procedure," Phys. Rev. A **9**, 1498 (1974).

⁴⁴C. F. Bunge, "Accurate determination of the total electronic energy of the Be ground state," Phys. Rev. A **14**, 1965 (1976).

⁴⁵E. Clementi, G. Corongiu, D. Bahattacharya, B. Feuston, D. Frye, A. Preiskorn, A. Rizzo, and W. Xue, "Selected topics in ab initio computational chemistry in both very small and very large chemical systems," Chem. Rev. **91**, 679 (1991).

⁴⁶A.-M. Mårtensson-Pendrill, S. A. Alexander, L. Adamowicz, N. Oliphant, J. Olsen, P. Öster, H. M. Quiney, S. Salomonson, and D. Sundholm, "Beryllium atom reinvestigated: A comparison between theory and experiment," Phys. Rev. A 43, 3355 (1991).

⁴⁷E. R. Davidson, S. A. Hagstrom, S. J. Chakravorty, V. M. Umar, and C. Froese Fischer, "Ground-state correlation energies for two- to ten-electron atomic ions," Phys. Rev. A 44, 7071 (1991).

⁴⁸C. Froese Fischer, "Convergence studies of MCHF calculations for Be and Li⁻,"
 J. Phys. B: At., Mol. Opt. Phys. 26, 855 (1993).

⁴⁹S. J. Chakravorty, S. R. Gwaltney, E. R. Davidson, F. A. Parpia, and C. Froese Fischer, "Ground-state correlation energies for atomic ions with 3 to 18 electrons," Phys. Rev. A 47, 3649 (1993).

⁵⁰ J. Komasa, W. Cencek, and J. Rychlewski, "Explicitly correlated Gaussian functions in variational calculations: The ground state of the beryllium atom," Phys. Rev. A **52**, 4500 (1995).

⁵¹ J. Noga, D. Tunega, W. Klopper, and W. Kutzelnigg, "The performance of the explicitly correlated coupled cluster method. I. The four-electron systems Be, Li⁻, and LiH," J. Chem. Phys. **103**, 309 (1995).

⁵²O. Jitrik and C. F. Bunge, "Atomic configuration interaction and studies of He, Li, Be, and Ne ground states," Phys. Rev. A 56, 2614 (1997).

J. Phys. Chem. Ref. Data 50, 043107 (2021); doi: 10.1063/5.0065282

⁵³H. K. G. Büsse and A. Lüchow, "Nonrelativistic energies for the Be atom: Double-linked hylleraas-CI calculation," Int. J. Quantum Chem. 66, 241 (1998).

⁵⁴J. Komasa, "Dipole and quadrupole polarizabilities and shielding factors of beryllium from exponentially correlated Gaussian functions," Phys. Rev. A 65, 012506 (2001).

⁵⁵K. Pachucki and J. Komasa, "Relativistic and QED corrections for the beryllium atom," Phys. Rev. Lett. 92, 213001 (2004).

⁵⁶K. Pachucki and J. Komasa, "Excitation energy of ⁹Be," Phys. Rev. A 73, 052502 (2006).

⁵⁷H. Nakatsuji, H. Nakashima, Y. Kurokawa, and A. Ishikawa, "Solving the Schrödinger equation of atoms and molecules without analytical integration based on the free iterative-complement-interaction wave function," Phys. Rev. Lett. **99**, 240402 (2007).

⁵⁸J. Toulouse and C. J. Umrigar, "Full optimization of Jastrow-Slater wave functions with application to the first-row atoms and homonuclear diatomic molecules," J. Chem. Phys. **128**, 174101 (2008).

⁵⁹S. Verdebout, P. Jönsson, G. Gaigalas, M. Godefroid, and C. Froese Fischer, "Exploring biorthonormal transformations of pair-correlation functions in atomic structure variational calculations," J. Phys. B: At., Mol. Opt. Phys. 43, 074017 (2010).

⁶⁰C. F. Bunge, "Configuration interaction benchmark for Be ground state," Theor. Chem. Acc. **126**, 139 (2010).

⁶¹ F. W. King, D. Quicker, and J. Langer, "Compact wave functions for the beryllium isoelectronic series, Li⁻ to Ne⁶⁺: A standard Hylleraas approach," J. Chem. Phys. **134**, 124114 (2011).

⁶² J. S. Sims and S. A. Hagstrom, "Hylleraas-configuration-interaction study of the ¹S ground state of neutral beryllium," Phys. Rev. A 83, 032518 (2011).

⁶³J. Komasa, R. Słupski, K. Jankowski, J. Wasilewski, and A. M. Teale, "High accuracy *ab initio* studies of electron-densities for the ground state of Be-like atomic systems," J. Chem. Phys. **138**, 164306 (2013).

⁶⁴S. Sharma, T. Yanai, G. H. Booth, C. J. Umrigar, and G. K.-L. Chan, "Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer," J. Chem. Phys. **140**, 104112 (2014).

⁶⁵J. S. Sims and S. A. Hagstrom, "Hylleraas-configuration-interaction nonrelativistic energies for the ¹S ground states of the beryllium isoelectronic sequence," J. Chem. Phys. **140**, 224312 (2014).

⁶⁶S. Bubin and L. Adamowicz, "Prediction of ¹P Rydberg energy levels of beryllium based on calculations with explicitly correlated Gaussians," J. Chem. Phys. **140**, 024301 (2014).

⁶⁷M. Przybytek and M. Lesiuk, "Correlation energies for many-electron atoms with explicitly correlated Slater functions," Phys. Rev. A 98, 062507 (2018).

⁶⁸S. Nasiri and M. Zahedi, "Quantum Monte Carlo simulations using Slater-Jastrow-backflow wave function," Comput. Theor. Chem. **1189**, 112978 (2020).

⁶⁹J. S. Sims, "Hylleraas-configuration interaction (Hy-CI) non-relativistic energies for the 3 ¹S, 4 ¹S, 5 ¹S, 6 ¹S, and 7 ¹S excited states of the beryllium atom," J. Res. Natl. Inst. Stand. Technol. **125**, 125006 (2020).

⁷⁰ M. Wang, G. Audi, F. G. Kondev, W. J. Huang, S. Naimi, and X. Xu, "The AME2016 atomic mass evaluation (II). Tables, graphs and references," Chin. Phys. C **41**, 030003 (2017).

⁷¹S. Bubin, M. Pavanello, W.-C. Tung, K. L. Sharkey, and L. Adamowicz, "Born–Oppenheimer and non-Born–Oppenheimer, atomic and molecular calculations with explicitly correlated Gaussians," Chem. Rev. **113**, 36 (2013).

⁷²M. Hamermesh, *Group Theory and its Application to Physical Problems* (Addison-Wesley, Reading, MA, 1962).

73 R. Pauncz, Spin Eigenfunctions (Plenum, New York, 1979).

⁷⁴S. Bubin and L. Adamowicz, "Energy and energy gradient matrix elements with *N*-particle explicitly correlated complex Gaussian basis functions with L = 1," J. Chem. Phys. **128**, 114107 (2008).

 75 S. Bubin and L. Adamowicz, "Explicitly correlated Gaussian calculations of the $^2P^o$ Rydberg spectrum of the lithium atom," J. Chem. Phys. **136**, 134305 (2012).

⁷⁶W. E. Caswell and G. P. Lepage, "Effective Lagrangians for bound state problems in QED, QCD, and other field theories," Phys. Lett. B 167, 437 (1986). ⁷⁷ K. Pachucki, "Effective Hamiltonian approach to the bound state: Positronium hyperfine structure," Phys. Rev. A 56, 297 (1997).

⁷⁸H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1977).

⁷⁹A. I. Akhiezer and V. B. Berestetskii, *Quantum Electrodynamics* (John Wiley & Sons, New York, 1965).

⁸⁰H. Araki, "Quantum-electrodynamical corrections to energy-levels of helium," Prog. Theor. Phys. **17**, 619 (1957).

⁸¹J. Sucher, "Energy levels of the two-electron atom to order α^3 Ry; ionization energy of helium," Phys. Rev. **109**, 1010 (1958).

⁸² P. K. Kabir and E. E. Salpeter, "Radiative corrections to the ground-state energy of the helium atom," Phys. Rev. **108**, 1256 (1957).

⁸³Z.-C. Yan and G. W. F. Drake, "Relativistic and QED energies in lithium," Phys. Rev. Lett. 81, 774 (1998).

⁸⁴K. Pachucki, "Simple derivation of helium Lamb shift," J. Phys. B: At., Mol. Opt. Phys. **31**, 5123 (1998).

 85 K. Pachucki, " $\alpha^4 R$ corrections to singlet states of helium," Phys. Rev. A 74, 022512 (2006).

⁸⁶J. Hiller, J. Sucher, and G. Feinberg, "New techniques for evaluating parityconserving and parity-violating contact interactions," Phys. Rev. A 18, 2399 (1978).

⁸⁷ R. J. Drachman and J. Sucher, "Annihilation in positron-atom collisions: A new approach," Phys. Rev. A 20, 442 (1979).

⁸⁸R. J. Drachman, "Nonrelativistic hyperfine splitting in muonic helium by adiabatic perturbation theory," Phys. Rev. A 22, 1755 (1980).

⁸⁹J. Hiller, J. Sucher, A. K. Bhatia, and G. Feinberg, "Parity-violating electricdipole transitions in helium," Phys. Rev. A **21**, 1082 (1980).

⁹⁰H. P. Trivedi, "Improved matrix elements of $\delta(r_1)$ using approximate wavefunctions," J. Phys. B: At., Mol. Opt. Phys. **13**, 839 (1980).

⁹¹ R. J. Drachman, "A new global operator for two-particle delta functions," J. Phys. B: At., Mol. Opt. Phys. **14**, 2733 (1981).

⁹²K. Pachucki, W. Cencek, and J. Komasa, "On the acceleration of the convergence of singular operators in Gaussian basis sets," J. Chem. Phys. **122**, 184101 (2005).

⁹³G. Drake and S. P. Goldman, "Bethe logarithms for Ps⁻, H⁻, and heliumlike atoms," Can. J. Phys. 77, 835 (2000).

⁹⁴M. Puchalski and K. Pachucki, "Relativistic, QED, and finite nuclear mass corrections for low-lying states of Li and Be⁺," Phys. Rev. A **78**, 052511 (2008).

⁹⁵Z.-C. Yan and G. W. F. Drake, "Theoretical lithium $2^2S \rightarrow 2^2P$ and $2^2P \rightarrow 3^D$ oscillator strengths," Phys. Rev. A **52**, R4316 (1995).

⁹⁶A. T. Bondy, D. C. Morton, and G. W. F. Drake, "Two-photon decay rates in heliumlike ions: Finite-nuclear-mass effects," Phys. Rev. A 102, 052807 (2020).

97 A. Edmonds, Angular Momentum in Quantum Mechanics, Princeton Landmarks in Mathematics and Physics (Princeton University Press, Princeton, NJ, 1996).

⁹⁸S. Bubin and L. Adamowicz, "Matrix elements of *N*-particle explicitly correlated Gaussian basis functions with complex exponential parameters," J. Chem. Phys. **124**, 224317 (2006).

⁹⁹S. Bubin and L. Adamowicz, "Computer program ATOM-MOL-nonBO for performing calculations of ground and excited states of atoms and molecules without assuming the Born–Oppenheimer approximation using all-particle complex explicitly correlated Gaussian functions," J. Chem. Phys. **152**, 204102 (2020).

¹⁰⁰I. Hornyák, L. Adamowicz, and S. Bubin, "Low-lying ²S states of the singly charged carbon ion," Phys. Rev. A **102**, 062825 (2020).

¹⁰¹ A. Kramida, Y. Ralchenko, J. Reader, and NIST ASD Team, NIST Atomic Spectra Database (version 5.8) (Online), 2020, available at http://physics.nist.gov/asd.

¹⁰²M.-K. Chen, "The energies and oscillator strengths of bound states of Be,"
 J. Phys. B: At., Mol. Opt. Phys. 31, 4523 (1998).

¹⁰³C. Froese Fischer and G. Tachiev, "Breit–Pauli energy levels, lifetimes, and transition probabilities for the beryllium-like to neon-like sequences," At. Data Nucl. Data Tables **87**, 1 (2004).

J. Phys. Chem. Ref. Data 50, 043107 (2021); doi: 10.1063/5.0065282

¹⁰⁴I. Martinson, A. Gaupp, and L. J. Curtis, "Comments on the Be I 2s²¹S – 2s2p¹P transition probability," J. Phys. B: At., Mol. Opt. Phys. 7, L463 (1974).

¹⁰⁵R. E. Irving, M. Henderson, L. J. Curtis, I. Martinson, and P. Bengtsson, "Accurate transition probabilities for the $2s^{21}S - 2s2p^{1}P$ transition in Be I and B II," Can. J. Phys. 77, 137 (1999).

 106 R. Schnabel and M. Kock, "*f*-value measurement of the Be I resonance line using a nonlinear time-resolved laser-induced-fluorescence technique," Phys. Rev. A **61**, 062506 (2000).

 107 D. Bégué, M. Mérawa, and C. Pouchan, "Dynamic dipole and quadrupole polarizabilities for the ground 2 1S and the low-lying 3 1S and 3 3S states of Be," Phys. Rev. A 57, 2470 (1998).

¹⁰⁸D. Bégué, M. Mérawa, M. Rérat, and C. Pouchan, "Dynamic scalar and tensor polarizabilities for the low-lying $2^{1}P^{o}$ and $2^{3}P^{o}$ states of Be," J. Phys. B: At., Mol. Opt. Phys. **31**, 5077 (1998).

¹⁰⁹ J. Mitroy, "Polarizabilities of the beryllium clock transition," Phys. Rev. A 82, 052516 (2010).