Extended Calculations of Energy Levels and Transition Rates for Singly Ionized Lanthanide Elements. I. Pr–Gd

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Abstract

Lanthanide elements play important roles as an opacity source in the ejected material from neutron star mergers. Accurate and complete atomic data are necessary to evaluate the opacities and to analyze the observed data. In this paper, we perform extended, ab initio atomic calculations from Pr II (Z = 59) to Gd II (Z = 64). By using multiconfiguration Dirac–Hartree–Fock and relativistic configuration-interaction methods, implemented in the general-purpose relativistic atomic structure package (GRASP2K), we calculate the energy levels and transition data of electric dipole transitions. These computations are based on strategies (with small variations) of Nd II published by Gaigalas et al. Accuracy of data is evaluated by comparing computed energy levels with the National Institute of Standards and Technology (NIST) database or other works. For the energy levels, we obtain the average relative accuracy of 8%, 12%, 6%, 8%, and 7% for Pr II, Pm II, Sm II, Eu II, and Gd II ions, respectively, as compared with the NIST data. Accuracy of energy transfer to the wavelength is 3%, 14%, and 11% for Pr II, Eu II, and Gd II. Our computed E1 type transition probabilities are in good agreement with experimental values presented by other authors especially for strong transitions.

Unified Astronomy Thesaurus concepts: Neutron stars (1108); R-process (1324); Gravitational wave sources (677); Atomic spectroscopy (2099); Transition probabilities (2074)

Supporting material: machine-readable tables

1. Introduction

Atomic opacities of heavy elements have a wide impact to astrophysics. In particular, recent observations of gravitational waves and electromagnetic waves from a neutron star merger (GW 170817; Abbott et al. 2017) highlight the needs for heavy-element opacities. In optical and infrared wavelengths, the electromagnetic counterpart of GW 170817 shows characteristics of kilonova emission powered by radioactive decays of newly synthesized r-process (or the rapid neutron capture process) nuclei. To study the r-process nucleosynthesis from the observed emission, we need to accurately understand the opacities of lanthanide elements since properties of a kilonova are mainly governed by bound–bound opacities of r-process elements and lanthanide elements give the largest contributions (Barnes & Kasen 2013; Kasen et al. 2013; Tanaka & Hotokezaka 2013).

Several works have been done to study the properties and opacities of lanthanide elements (Kasen et al. 2013; Fontes et al. 2017; Tanaka et al. 2018, 2019). However, atomic calculations to evaluate the total opacities are not necessarily accurate enough to give a wavelength and a transition probability of each transition (Tanaka et al. 2019). Recently, Watson et al. (2019) reported identification of Sr in the spectra of a kilonova associated with GW 170817. In principle, other elements can also be identified in the spectra. However, the line list used for astrophysics is not necessarily complete even for strong transitions—in particular, in infrared wavelengths. By these reasons, it is still not straightforward to fully decode the spectra of a kilonova. Accurate atomic calculations of lanthanide elements, therefore, play an important role as a benchmark to give accurate atomic data (Gaigalas et al. 2019). There are many semi-empirical works that provide accurate atomic data of the lanthanide elements. In these works, the Racah–Slater parametric method is used (Wyart 2011). This method is known to give an excellent agreement between calculated energies using fitted radial parameters and available experimental energies. However, correct level identification of experimental spectra is needed, which is not always available. On the other hand, ab initio methods can provide complete atomic data set without any empirical parameter. Nevertheless, there are few applications of such ab initio methods for lanthanide with spectroscopic accuracy. This is because systematic improvement of subtle correlation effects in complicated atomic structures of open-4f shell is not studied thoroughly.

In our previous paper (Gaigalas et al. 2019), we performed accurate calculations for Nd ions. In this paper, we extend our calculations to Pr II, Pm II, Sm II, Eu II, and Gd II. Namely, we perform energy spectrum computations for states of the following configurations: [Xe]4f⁶⁶⁶ {6s, 5d, 6p} and [Xe]4f⁶⁷⁷ {5d6s, 5d6p, 6s6p, 5d²} for N = 3, 5, 6, 7, and 8. We also perform energy spectrum computations for states of [Xe]4f⁶⁸⁸ configuration for Sm II and Eu II and [Xe]4f⁶⁷⁶² configuration for Gd II. Levels up to 10 eV are computed since such low-lying energy levels play dominant roles in the opacities in the neutron star merger ejecta at typical temperature of 5000 K (Gaigalas et al. 2019). Using these results, electric dipole (E1) transitions data were computed between these states. In this paper, we aim at providing complete atomic data (all levels up to 10 eV of mentioned configurations and all E1 type transition between them), with the overall accuracy for the energy level at about 10%. This accuracy is not high enough to directly compare with spectroscopic experiments.
but it is adequate to evaluate the opacities ("opacity accuracy" rather than "spectroscopic accuracy"; Gaigalas et al. 2019). In fact, typical accuracy of complete atomic calculations (Kasen et al. 2013; Tanaka et al. 2018) is much lower than the accuracy presented in this paper.

The calculations are done using multiconfiguration Dirac–Hartree–Fock (MCDHF) and relativistic configuration-interaction (RCI) methods (Grant 2007; Fischer et al. 2016), which are implemented in the general-purpose relativistic atomic structure package (GRASP2K; Jönsson et al. 2013). We employ a strategy similar to that of Gaigalas et al. (2019), including electron correlation, which is suitable for series of rare earth ions. For low-lying levels, higher accuracy can be achieved using computational schemes, including more electron correlations as in Radžiūtė et al. (2015). In addition, there is an advantage in the computation since large computational tasks can be split into smaller tasks by using this method.

In Section 2, we describe our method and strategy of calculations. Then, we show results of energy level structure and transition probabilities in Sections 3 and 4, respectively. Finally, we give summary in Section 5.

2. Methods

2.1. Computational Procedure

The computational methods used in this paper follow the methods used in Gaigalas et al. (2019). Therefore, we briefly outline the methods in this section. We refer the reader to Fischer et al. (2016) for further details. We use the MCDHF method, based on Dirac–Coulomb Hamiltonian, in this work. The atomic state functions (ASFs) are expressed by a linear combination of symmetry adapted configuration state functions (CSFs). The CSFs are built from products of one-electron Dirac orbitals. The radial parts of the Dirac orbitals and the expansion coefficients are optimized to self-consistency in the relativistic self-consistent field procedure.

The spin-angular approach (Gaigalas & Rudzikas 1996; Gaigalas et al. 1997) is used in these computations. The approach is based on the second quantization in a coupled tensorial form, on the angular momentum theory in the orbital, spin, and quasispin spaces and on the reduced coefficients of the fractional parentage. It allows us to study configurations with open f-shells without any restrictions.

In the following RCI calculations, the Breit interaction is included in the Hamiltonian. In the RCI calculation, the leading quantum electrodynamics corrections (QEDs), self-interaction, and vacuum polarization are also included.

The label of the ASF is the same as the label of the dominating CSF. The ASFs are obtained as expansions over jj-coupled CSFs. To provide the ASFs in the LSJ labeling system, transformation from a jj-coupled CSF basis to an LSJ-coupled CSF basis has been done (Gaigalas et al. 2017). A review of all these methods and on the GRASP2K package can be found in Fischer et al. (2016).

2.2. Computation of Transition Probabilities

For electric dipole transitions, there are two forms of the transition operator: the length (Babushkin) and velocity (Coulomb) forms. Although the exact solutions of the Dirac equation should give the same value of the transition moment (Grant 1974), they do not necessarily agree in numerical calculations. The quantity of \( dT = |A_l - A_s|/\max(A_l, A_s) \) (Ekman et al. 2014) defines the accuracy of the computed transition rates, where \( A_l \) and \( A_s \) are the transition rates in length and velocity forms, respectively.

The calculation of the transition moment breaks down in the task of summing up reduced matrix elements between different CSFs. Using standard techniques, by assuming that both left and right hand CSFs are formed from the same orthonormal set of spin orbitals, the reduced matrix elements can be evaluated. This constraint is severe, since a high-quality and compact wave function requires orbits optimized for a specific electronic state (see, for example, Fritzche & Grant 1994).

To avoid the problems of having a single orthonormal set of spin orbitals, the wave function representations of the two states are transformed in a way that the orbital sets became biorthonormal (Olsen et al. 1995). To evaluate the matrix elements of the transformed CSFs, standard methods, as in Fischer et al. (2016), are used.

2.3. Computational Schemes

To compute singly ionized lanthanide elements, the strategy C by Gaigalas et al. (2019) is used. Details of this strategy and the extension of it are given below. The active space method is used for computation of energy levels and E1 transitions. The configuration space is increased step by step, by increasing the number of layers (L)—that is, a set of virtual orbitals. The virtual orbitals of the increased layer are optimized in the relativistic self-consistent field procedure, while all orbitals of inner layers are fixed. The scheme used to increase the active spaces of the CSFs is presented below:

\[
\begin{align*}
\text{AS}_{0L} &= \{6s, 6p, 5d\}, \\
\text{AS}_{1L} &= \text{AS}_{0L} + \{7s, 7p, 6d, 5f\}, \\
\text{AS}_{2L} &= \text{AS}_{1L} + \{8s, 8p, 7d, 6f, 5g\}.
\end{align*}
\]

The number of computed levels and CSFs in the final even and odd state expansions are presented in Table 1.

Computations are performed for each configuration separately (the single reference method). This method allows us to split the large computations into several tasks. In each task, the wave function expansion for a single reference configuration is constructed by substitution of one and two electrons from the reference configuration. For configurations \( 4f^N \) \( 6s, 4f^{N-1}6p, \) and \( 4f^{N-1}5d, \) single and/or double (SD) substitutions are allowed from \( 4f^Nnl \) shells \((l = s, p, \) and \( d)\) to \( \text{AS}_{0L,1L} \) and single (S) substitutions are allowed for \( \text{AS}_{2L}. \) For configurations \( 4f^{N-1}5d6s, 4f^{N-1}5d6p, 4f^{N-1}6s6p, \) and \( 4f^{N-1}5d^2, \) only S substitutions are allowed. For Sm II and Eu II ions, a new configuration \( 4f^{N+1} \), which was not taken into account in the
strategy C of Gaigalas et al. (2019), is computed. For this configuration, single, double, and triple (SDT) substitutions are allowed from $4f^{N+1}$ shell to $AS_{4d,1l}$ and SD substitutions are allowed to $AS_{2l}$. For configuration $4f^{N-1}nl^m l''$, two electrons are excited from $4f$ orbital, and for $4f^N nl$, only one electron is excited from $4f$ orbital. Therefore, to include compensated correlations, we need to make less excitations from the first configuration and more excitations from the second one. For example, if we do SD substitutions for the $4f^{N-1}nl^m l''$ configuration, we need to make SDT substitutions for the $4f^N nl$ configuration.

To compute energy levels, it is important to have correct core radial wave functions—that is, initial Dirac–Fock computations. Correct selection of the core stabilizes solution of self-consistent field computation. We find that core radial wave functions $[Xe]4f$ from the ground configuration $[Xe]4f^66s$ are the best solution. Radial wave functions up to the $4f$, $5s$, $5p$ orbital are taken from the ground configuration for these configurations $4f^{N-1}5d6s$, $4f^{N-1}5d6p$, $4f^{N-1}6s6p$, and $4f^{N-1}5d^2$. Meanwhile, the radial wave functions were computed for each configurations of $4f^N nl$ ($l = s, p, d$) separately.

For neutral atoms and ions of lanthanide elements with different ground configurations, we suggest that their ground configuration radial wave functions are used as a common core. For example, for neutral lanthanides, radial wave functions of the ground configurations $[Xe]4f^66s^2$ can be used as a common core.

For Eu II and Gd II, the wave function is investigated differently due to the rapid increase of the number of CSFs in the active space (see Table 1). For these ions, self-consistent field computations are performed not for all $J$ values but only for one $J$ value. Then, using computed radial wave functions, RCI computations are performed. For example, for the configuration of Eu, $4f^56s$ atomic states only with $J = 4$ are computed and it is later used in the RCI computation for $J = 0$–13. For all configurations, the lowest $J$ values are selected for computation of the radial wave functions. This computational method demands less computational resources.

In addition, some states of the Rydberg series (up to 10 eV) are computed for Eu II. This includes 38 levels from configurations $4f^6 \{7s, 8s, 6d, 7d, 7p, 8p\}$. Radial wave functions for configurations $4f^6 \{7s, 8s\}$ up to $4f$ are taken from the ground configuration ($4f^66s$). For the rest configurations, radial wave functions are computed in the same manner as in the configurations $4f^6 \{5d, 6p\}$. This means that each configuration from $4f^6 \{6d, 7d, 7p, 8p\}$ has different radial wave functions. Active space generated in a similar manner as for the configurations $4f^66s, 5d, 6p$. For example, active space for the configuration are generated by SD substitutions from $4f^6 8s$ to $AS_{4d} = \{6p, 5d\}$ and $AS_{2l} = AS_{4d} + \{6s, 7p, 6d, 5f\}$ and by S substitutions to $AS_{2l} = AS_{4d} + \{7s, 8p, 7d, 6f, 5g\}$.

For Gd II, the radial wave function is generated also for only one $J$ value. Radial wave functions of $4f^75d^2$, $4f^76s^2$, $4f^75d6s$, and $4f^66p$ are computed together, using radial wave function of configuration $4f^76s$ up to $4f$. The rest of the configurations are computed in the same manner as for Eu II. The MCDHF calculations are then followed by RCI calculations by including the Breit interaction and leading QED effects. The same active space ($AS_{4d}$) is used for the RCI computations as well as for MCDHF calculations.

### 3. Energy Levels

All levels for $Z = 59$–64 ions are given in Figure 1, and the energy data computed for Pr II, Pm II, Sm II, Eu II, and Gd II are given in machine-readable format in Tables 2–7, respectively. This includes the label, $J$ and $P$ values, and energy value. Levels are given in LS-coupling, although it is suitable only for the lowest states of configurations and determination the configuration is complicated for higher states (Cowan 1981).

For the labels, we use notation $4f^{N-}(2S+1)L n^m^l (2S+1)L'$. Intermediate quantum numbers define parent levels of $4f^{N-}(2S+1)L$, where $N$ is electron number in $4f$ shell, $(2S+1)$ is multiplicity, $N_r$ is a sequential index number representing the group labels $iWU$ for the term, $(J$ is seniority quantum number, $W$ is label of parameters $(w_1, w_2, w_3)$ and represents $R_7$ group, $U$ is label of parameters $(u_1, u_2)$ and represents $G_2$ group), and $L$ is orbital quantum number (see Gaigalas & Radzakis 1998 for more about $N_r$). More complicated configurations are presented in the similar way.

To evaluate the accuracy of our calculations, comparison with critically evaluated data is necessary. In this section, we first summarize the available data for energy levels of Pr II, Pm II, Sm II, Eu II, and Gd II in the National Institute of Standards and Technology (NIST) database. Then, we compare calculated energy levels with these available data.

#### 3.1. Available Data

##### 3.1.1. Pr II

Ginibre (1989a) investigated 105 odd and 187 even experimental energies based on Fourier transform (FT) spectroscopy in the range of 2783–27,920 cm$^{-1}$. Also, the large number levels were investigated by Rosen et al. (1941) and Blaise et al. (1973, 1974). They performed a semi-empirical fitting procedure to assign some levels in the LS-coupling (Ginibre 1989b). Later, Ivarsson et al. (2001) presented improved 39 energy levels using FT spectroscopy in the 2800–8000 Å region. Furmann et al. (2001, 2005, 2007) investigated 31 odd and 14 even levels, using laser-induced fluorescence (LIF) spectroscopy in a hollow cathode discharge lamp. More recently, Akhtar & Windholz (2012) redetermined energy values of 227 levels (74 odd and 153 even parity) and hyperfine structures of 477 transitions in the range of 3260–11,700 Å. They corrected the energy levels from the works of Ginibre (1989a) and Ivarsson et al. (2001).

All of these levels are measured/reanalyzed in high accuracy. However, each work presents energy levels in a narrow range as shown in Figure 2. Therefore, the transitions between measured energy levels give a too small number of lines needed for computation of opacities in neutron star mergers. Data of these authors are summarized by Martin et al. (1978). Since the NIST database (Kramida et al. 2018) includes the work by Martin et al. (1978), we only give comparison with the NIST database here.

##### 3.1.2. Pm II

Pm II is one of the ions whose spectrum is not well investigated. Energy levels of two configurations, $4f^66s$ and $4f^55d$, were investigated by Martin et al. (1978). Five new levels of $4f^55d$ configuration were measured by Ottot et al. (1995) with the collinear laser ion beam spectroscopy method and were identified using the Hartree–Fock method.
3.1.3. Sm II

Albertson (1936) assigned terms of 40 even levels of the $4f^66s$ and $4f^65d$ configurations based on the Zeeman patterns of over 300 lines. Spector (1970a) did semi-empirical computation of energy values and LS-composition of 55 levels for $4f^6(7F)5d$ configuration. Also, a large amount of work for energy levels was...
done by Blaise et al. (1969): 325 levels for Sm II were obtained from the Zeeman effect measurement in the visible and the ultraviolet spectrum. Then, these energy levels were re-evaluated by Martin et al. (1978). Rao et al. (1990) attempted to identify odd configurations for some levels using isotope shifts data, which was carried out on a recording Fabry–Perot spectrometer. The hyperfine structure and isotope shift were also measured by collinear fast-ion beam laser spectroscopy. These data were used to assign configurations to the 13 odd upper levels by Villemoes et al. (1995). Note that some of them do not have identifications by Martin et al. (1978).

### 3.1.4. Eu II

Configurations $4f^7(6s, 7s, 8s, 8p, 5d, 6d, 6p)$, $4f^65d6s$, and $4f^65d^2$ for 156 levels were resolved with the spark spectrum of

| No. | Label | J | P | E |
|-----|-------|---|---|---|
| 1   | $4f^7(6s) 6s 3H$ | 2 | – | 0.00 |
| 2   | $4f^7(6s) 6s 3H$ | 3 | – | 441.78 |
| 3   | $4f^7(6s) 6s 3H$ | 4 | – | 1073.15 |
| 4   | $4f^7(6s) 6s 3H$ | 5 | – | 1850.51 |
| 5   | $4f^7(6s) 6s 3H$ | 6 | – | 1858.38 |
| 6   | $4f^7(6s) 6s 3H$ | 7 | – | 2765.09 |
| 7   | $4f^7(6s) 6s 3H$ | 8 | – | 2830.31 |
| 8   | $4f^7(6s) 6s 3H$ | 9 | – | 3765.53 |
| 9   | $4f^7(6s) 6s 3H$ | 10 | – | 3914.91 |
| 10  | $4f^7(6s) 6s 3H$ | 11 | – | 4799.46 |
| 11  | $4f^7(6s) 6s 3H$ | 12 | – | 4836.02 |
| 12  | $4f^7(6s) 6s 3H$ | 13 | – | 5078.38 |
| 13  | $4f^7(6s) 6s 3H$ | 14 | – | 5507.08 |
| 14  | $4f^7(6s) 6s 3H$ | 15 | – | 6298.26 |
| 15  | $4f^7(6s) 6s 3H$ | 16 | – | 6322.77 |
| 16  | $4f^7(6s) 6s 3H$ | 17 | – | 6567.93 |
| 17  | $4f^7(6s) 6s 3H$ | 18 | – | 6678.52 |
| 18  | $4f^7(6s) 6s 3H$ | 19 | – | 6917.29 |
| 19  | $4f^7(6s) 6s 3H$ | 20 | – | 7232.66 |

(This table is available in its entirety in machine-readable form.)
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Table 6
Energy Levels (in cm$^{-1}$) Relative to the Ground State for the States of Gd II

| No. | Label | $J$ | $P$ | $E$ |
|-----|-------|-----|-----|-----|
| 1   | $4f^7(5S) 5d  (^D)6s$ | 5/2 | –   | 0.00 |
| 2   | $4f^7(5S) 5d  (^D)6s$ | 7/2 | –   | 225.02 |
| 3   | $4f^7(5S) 5d  (^D)6s$ | 9/2 | –   | 536.90 |
| 4   | $4f^7(5S) 5d  (^D)6s$ | 11/2 | – | 959.98 |
| 5   | $4f^7(5S) 5d  (^D)6s$ | 13/2 | – | 1536.81 |
| 6   | $4f^7(5S) 5f^2(F) 10F$ | 3/2 | – | 3026.08 |
| 7   | $4f^7(5S) 5f^2(F) 10F$ | 5/2 | – | 3173.49 |
| 8   | $4f^7(5S) 5f^2(F) 10F$ | 7/2 | – | 3382.26 |
| 9   | $4f^7(5S) 5f^2(F) 10F$ | 9/2 | – | 3654.80 |
| 10  | $4f^7(5S) 5d  (^D)6s$ | 3/2 | – | 3767.49 |
| 11  | $4f^7(5S) 5d  (^D)6s$ | 5/2 | – | 3965.84 |
| 12  | $4f^7(5S) 5f^2(F) 10F$ | 11/2 | – | 3994.44 |
| 13  | $4f^7(5S) 5d  (^D)6s$ | 7/2 | – | 4269.62 |
| 14  | $4f^7(5S) 5f^2(F) 10F$ | 13/2 | – | 4405.08 |
| 15  | $4f^7(5S) 5d  (^D)6s$ | 9/2 | – | 4713.57 |
| 16  | $4f^7(5S) 5f^2(F) 10F$ | 15/2 | – | 4888.14 |
| 17  | $4f^7(5S) 5d  (^D)6s$ | 11/2 | – | 5359.77 |
| 18  | $4f^7(5S) 6s^2 5s$ | 7/2 | – | 5713.88 |
| 19  | $4f^8(F) 6s 8F$ | 13/2 | + | 7507.66 |
| 20  | $4f^8(F) 6s 8F$ | 11/2 | + | 8691.73 |

(This table is available in its entirety in machine-readable form.)

arc by Russel et al. (1941). This work is the extension of the analysis by Albertson (1934) on nine levels of $4f^7(6s, 5d, 6p)$ configurations. Then, these energy levels were re-evaluated by Martin et al. (1978). More recently, 13 new energy levels of $4f^7(6s)$ configuration were suggested from hyperfine constant and isotope shift measurements (Furmann & Stefańska 2013).

3.1.5. Gd II

Albertson et al. (1940) investigated 9 odd and 11 even energy levels, deduced quantum numbers from Zeeman effect pattern, and established the ground configurations to be $4f^75d6s$. Venugopalan et al. (1998) and Ahmad et al. (1979) the measured isotope shift of 33 spectroscopic lines, using a photoelectric recording Fabry–Perot spectrometer. They suggested new configuration identifications of four high energy levels (lying above 35,000 cm$^{-1}$): 35,362.630 cm$^{-1}$ ($J = 13/2$) as $4f^75d6s$, 35,822.697 cm$^{-1}$ ($J = 9/2$) as mix of two configurations $4f^75d6s+4f^86p$, and 37,831.032 cm$^{-1}$ ($J = 11/2$) and 38,010.603 cm$^{-1}$ ($J = 11/2$) as $4f^86p$. Blaise et al. (1971) did the analysis of the spark spectrum of Gd II of 178 new levels. A total of 30 levels were ascribed to the $4f^8(F)6p$ configuration by their strong transitions with the levels on the $4f^8(F)6s$ and $4f^8(F)5d$ subconfigurations. Spector (1970a) did semi-empirical computation of energy values and LS-composition of 57 levels for $4f^8(F)5d$ configuration. Martin et al. (1978) listed 164 odd and 150 even parity energy levels of Gd II. Spector (1970b) did an extended analysis of the levels of $4f^8(F)6s, 6p, 5d$ configurations and measured new levels of $4f^8(F)6s, 5d$ configurations and new odd levels.

3.2. Comparison of the Energy Levels

The energy levels for each configuration are compared with those in the NIST database in Figure 1. Only the common configurations for Pr II–Gd II are presented in the figure. Although the energy levels in the NIST database sometimes include questionable identification of the configuration, this figure includes all levels.

To analyze the accuracy of our calculations as compared with the NIST data, we use an expression $\Delta E_i/E_{\text{NIST}} = (E_{\text{NIST}} - E_i)/E_{\text{NIST}} \times 100\%$. For the indicator of the accuracy for many levels, we use a value $\Delta E/E = \sum_i^{N} |\Delta E_i|/E_{\text{NIST}}$, where $N$ is the number of the compared levels. A summary of the accuracy for each configuration is given in Table 7. Levels with clear identification are included into the comparison. An empty space in Table 7 means that configuration is not computed while those with “—” mean that data are missing in the NIST database (or there is only one level). The last line (all) of the table presents averaged accuracy with clear identification between our results and the NIST database.

Overall, we find that our calculations give good accuracy: 8%, 12%, 6%, 8%, and 7% for Pr II, Pm II, Sm II, Eu II, and Gd II ions, respectively. There is no clear trend with the atomic number Z. The accuracy depends on the configurations. For example, the degree of agreement for the $4f^86s, 4f^75d$, and $4f^86p$ configurations slightly differ. These variations of the differences are mainly caused by the different number of levels used for comparison. Note that the biggest deviation is found for level $5S_7/2$ of configuration $4f^76s^2$ (66% difference for this one level).

As mentioned in Section 2.3, computations of Eu II are performed in a slightly different manner: radial wave functions are computed only for one $J$ symmetry of the lowest ASF. To test the influence of such splitting, we compute configurations $4f^76s, 4f^75d, 4f^65d6s, 4f^65d6p$, and $4f^55d2$ in both ways. We find that the differences between two methods are small: the maximum averaged difference of energy levels per configuration is 0.5% for $4f^75d$ configuration (614 levels) and the minimum difference is 0.02% for $4f^76s$ (261 levels). Levels of the Rydberg state of the configurations $4f^7(7s, 8s, 6d)$ for Eu II are also compared in Table 7. There is a good agreement for levels of configurations of $4f^7(7s, 6d)$ obtained in this research with values from the NIST database.
The accuracy of our calculations can also be evaluated using Figure 3, which shows the energy difference between the lowest levels of \(4f^{N-1}5d6s\) and the lowest levels of \(4f^{N}6s\) configurations for singly ionized lanthanides. As shown in the figure, the overall agreement is very good. Our results and those in the NIST database give smaller energy differences than those in Martin (1971) and Cowan (1981) for Nd II and Pm II ions. The increase of the energy difference is observed for Eu II by all of the works, but our result shows a bigger increase than in Martin (1971), Cowan (1981), and the NIST data.

Here, it should be noted that, for the cases of Pr II and Sm II, the identification of \(4f^{N-1}5d6s\) configurations are questionable in the NIST database. A more detailed investigation was done by Brewer (1971, see their Figure 1). They estimated energies for the lowest levels of configurations involving \(4f, 5d, 6p,\) and \(6s\) shells for singly-triply ionized lanthanides and actinides. Their computations are based on the thermodynamic data of the metals. In a similar manner, the energy differences were also analyzed by Vander Sluis & Nugent (1974). In fact, our results are very close to the data of these authors.

### 3.3. Energy Level Distribution for Each Configuration

Identification of energy levels is a complicated task for lanthanides due to a mix of configurations. Even assigning particular configuration labeling to some levels is complicated. The discussion below should give enlightenment on the inner structure of the energy spectrum. Energy levels formed groups around parent level of \(4f^{N}\) or \(4f^{N-1}\) configurations with the same term of \(f\) shell. Levels belonging to the different groups are separated by energy gaps. Below are given more details about these groups for each configuration.

Energy level structures for states of \(4f^{N}\) \((6s, 6p, 5d),\) \(4f^{N-1}\) \((5d6s, 5d6p, 6s6p),\) and \(4f^{N-1}d2\) configurations are presented in Figure 1. The cut off line of 80,700 cm\(^{-1}\) (10 eV) is given by the horizontal lines. For Pr II and Nd II, computations are done up to ionizations limits: 85,745 cm\(^{-1}\) for Pr II and 86,970 cm\(^{-1}\) for Nd II according to the NIST database. The number of computed levels are displayed below the line and the number of levels above the line are left uncomputed. The sum of these numbers comprise a possible number of levels in \(jj\)-coupling. We find that the increase of the nuclear charge has a small effect on the positions of the first level relative to the ground state for the configurations \(4f^{N}6p\) and \(4f^{N}5d\). The energy level structures of these configurations are influenced by the structure of core \([X]4f^{N}\). Similar to the system difference analyzed by Cowan (1981), the increase of the energy of the first level relative to the ground state is found for the configurations of \(4f^{N-1}5d6s, 4f^{N-1}5d6p, 4f^{N-1}s6p,\) and \(4f^{N-1}d2\) (see Figure 3 for \(4f^{N-1}5d6s\)). The highest density of the energy levels are found for \(4f^{N-1}d2\) and \(4f^{N-1}5d6p\) configurations.

The lowest levels of the \(4f^{N}6s\) and \(4f^{N}6p\) configurations form blocks of energy levels around the parent levels of \(4f^{N}\) \((\frac{1}{2}f^0), (\frac{3}{2}f^0), (\frac{3}{2}f^0), (\frac{5}{2}F^0), (\frac{3}{2}S^0'), (\frac{5}{2}P^0), (\frac{3}{2}I^0),\) and \((\frac{3}{2}D^0)\) for \(Z = 59–64,\) respectively. After the levels with a core configuration marked by "**\" above, there is an energy gap, except for \(4f^{7}6p\) of the Pr II ion. Levels with the specific parent levels do not mix with others, except for the parent level states of \(4f^{7}6p\) of the Pr II ion \(4f^{7}6H\) mix between \(4f^{7}5F^0\). For the \(4f^{7}5d\) configuration, the situation is different because of the strong interaction between \(4f\) and \(5d\) (Figure 1).

For the \(4f^{N-1}5d6s\) configuration, groups of energy levels formed around the lowest parent levels for only two elements, i.e., Eu II and Gd II. These parent levels are \(4f^{6}7F^0\) and \(4f^{7}5S^0\) for Eu II and Gd II, respectively. For \(4f^{N-1}5d6p\) configuration, only Gd II has formed a group of energy levels around the \(4f^{7}5S^0\) parent level (Figure 1).

Levels of the \(4f^{N-1}s6p\) configuration do not form a group of energy levels around the parent levels. For Eu II, all levels of \(4f^{6}7s6p\) and of \(4f^{5}5s6p\) configurations belong to the parent levels of \(4f^{6}7F^0\) because of the 10 eV cut off (Figure 1). For the \(4f^{N-1}d2\) configuration, groups of energy levels form around the lowest parent levels for Gd II \(4f^{8}5S^0\) (Figure 1).

Radii of the orbitals of the configurations \(4f^{N}6s\) and \(4f^{N-1}5d6s\) are presented in Table 8. For higher Z, all orbitals contract (see Table 8). The exceptions are Eu II and Gd II: there are no big differences for the \(5d_{\pm}\) and \(5d_{\mp}\) orbitals between Eu II and Gd II. Indeed, for Gd II, the radii for orbitals \(5d_{\pm}\) and \(5d_{\mp}\) show a small increase with respect to Eu II. This may be caused by different computations of the radial wave functions (see Section 2.3). Some of the radii are compared with computations by Indelicato et al. (2007; [107]). Radii by

### Table 7

Comparison of Energy Levels with the NIST Database, \(\Delta E/E\) (in %) and the Number of Compared Levels (NL)

|     | Pr II | Nd II | Pm II | Sm II | Eu II | Gd II |
|-----|-------|-------|-------|-------|-------|-------|
| \(4f^{N}6s\) | 6     | 7     | 15    | 27    | 13    | 17    |
| \(4f^{N}6p\) | 4     | 12    | 13    | 23    | ...   | ...   |
| \(4f^{N}5d\) | 10    | 33    | 8     | 47    | 10    | 5     |
| \(4f^{N-1}5d6s\) | ...   | ...   | ...   | ...   | 15    | 8     |
| \(4f^{N-1}5d6p\) | ...   | ...   | ...   | ...   | ...   | ...   |
| \(4f^{N-1}6s6p\) | ...   | ...   | ...   | ...   | 3     | 2     |
| \(4f^{N-1}6d\) | ...   | ...   | ...   | ...   | 9     | 1     |
| All   | 8     | 53    | 10    | 158   | 12    | 22    |

Note. Nd II data are published in Gaigalas et al. (2019). Levels with clear identification are included into the comparison.
In the following sections, we compare the calculated transition probabilities with available data, except for Prm II for which there is not enough available data.

4.1. Pr II

For Pr II, rather rich data are available in the NIST database. Therefore, it can be used as an evaluation of our calculations. Comparison between the calculated E1 transitions probabilities and those in the NIST database is presented in Figure 4. Figure 4 includes transitions between 4f3 6s and 4f3 6p and transitions between 4f3 6p and 4f3 5d with a clear level identification. The same transitions in the length and velocity form are connected with dashed lines. Transitions in the NIST database are based on FT spectroscopy by Ivarsson et al. (2001) and measurements of branching fractions (BF) with the use of a laser/fast-ion-beam method by Li et al. (2007) and lifetimes determined in a previous study with the beam laser method (Scholl et al. 2002a).

We find that transition probabilities calculated in two forms agree better for the transitions between 4f3 6s and 4f3 6p than those between 4f3 6p and 4f3 5d. Compared with the data by other authors, our transitions in the velocity form give a better agreement in the strong transition area. Therefore, hereafter, we show transition probabilities computed in the velocity form.

As for the transition wavelength, our calculations give a good agreement with the NIST data. Averaged agreement in the transition wavelength is 2% for the transitions between the states of configurations 4f3 6s and 4f3 6p and 4% for the transitions between the states of configurations 4f3 6p and 4f7 5d (see Figure 5).

4.2. Sm II

Xu et al. (2003) performed radiative lifetime measurements with time-resolved LIF techniques for 47 levels and performed relativistic Hartree–Fock computations over the energy range of 21,000–36,000 cm⁻¹, but again, the identification of these levels is unclear. Large amount of data (958 lines) have been measured with the same method (Lawler et al. 2006), but all upper levels do not have clear identification. Lifetimes of 82 levels in the range of 21,655.420–29,591.120 cm⁻¹ were investigated by the beam laser method and transition probabilities were calculated using branching ratios for 35 transitions by Scholl et al. (2002b).

For Sm II, there are transitions probabilities for seven lines in the NIST database. Unfortunately, upper levels do not have clear identification of the configuration. However, for the purpose of comparison of the transition probabilities, we suggest identifications of the levels, as shown in Table 14. This identification is based on the results displayed in Figure 1 (sections 5d6s, 6p, and 5d²) and the machine-readable Table 4.

Levels of the following configurations—4f²5d6s, 4f²5d², 4f⁷ 6p, and 4f⁷—have similar starting positions (the lowest configuration is 4f⁷5d²). This was also confirmed by Xu et al. (2003, see their Figure 3). Meanwhile, according to our study, the lowest energy levels with J = 1/2 for configurations 4f⁷ 6p, 4f⁷ 5d6s, 4f⁷ 5d², and 4f⁷ are at 21,418; 24,889; 26,022; and 44,621 (in cm⁻¹), respectively. Therefore, the lowest energy level with J = 1/2 belongs to the configuration 4f⁷ 6p and the first four levels (4G1/2, 4D3/2, 4F5/2, and 4F3/2) with energies 21,418; 21,892; 24,403; and 25,378 (in cm⁻¹) were assigned to the 4f⁷ 6p configuration (see Table 14).

### Table 8

| Ion | (4f)⁷ | (4f)⁶ | (5d)⁷ | (5d)⁶ | (6s)⁴ |
|-----|-------|-------|-------|-------|-------|
| Pr II | 1.0833 | 1.0986 | 2.5036 | 2.5484 | 4.3130 |
| I07  | 1.0589 | 1.0667 | ...    | ...    | 4.2924 |
| Nd II | 1.0291 | 1.0440 | 2.4607 | 2.5085 | 4.2252 |
| I07  | 1.0054 | 1.0190 | ...    | ...    | 4.2252 |
| Pm II | 0.9832 | 0.9981 | 2.4223 | 2.4717 | 4.1948 |
| I07  | 0.9624 | 0.9796 | ...    | ...    | 4.1608 |
| Sm II | 0.9442 | 0.9590 | 2.3892 | 2.4400 | 4.1402 |
| I07  | 0.9249 | 0.9392 | ...    | ...    | 4.1012 |
| Eu II | 0.9098 | 0.9256 | 2.3642 | 2.4272 | 4.0870 |
| I07  | 0.8920 | 0.8999 | ...    | ...    | 4.0438 |
| Gd II | 0.8797 | 0.8929 | 2.3991 | 2.5041 | 3.6878 |
| I07  | 0.8218 | 0.8221 | 2.4547 | 2.4846 | 3.7930 |

Note.

* Orbital radii of Nd II were computed during MCDHF computations in Gaigalas et al. (2019) but have not been published.

Indelicato et al. (2007) differ from 1%–8% from those computed in this paper. It is likely that these differences are caused by inclusion of Breit interaction into the self-consistent field procedure in the MCDHF computations.

### 4. E1 Transitions

In this section, we show the results of our calculations of transitions probabilities. The transition data computed for Pr II, Pm II, Sm II, Eu II, and Gd II are given in machine-readable format in Tables 9–13. The tables include identification of upper and lower levels in the LSJ coupling, transition energy, wavelength, line strength, weighted oscillator strength, and transition probabilities in the length form. The numbers of transitions are 411,314; 7,104,005; 4,720,626; 4,67,724 (plus 13,154 transitions with Rydberg states, 480,878 in total); and 1,383,694 for Pr II, Pm II, Sm II, Eu II, and Gd II, respectively.
Table 9

| Lower State | Upper State | $\Delta \varepsilon$ (cm$^{-1}$) | $\lambda$ (Å) | $\sigma$ | $g_f$ | $A$ (s$^{-1}$) | $dT$ |
|-------------|-------------|-------------------------------|--------------|-------|-------|---------------|------|
| $4^3P^2(5S) 3D_1$ | $4^1P^0(5D) 3P_0$ | 36101 | 9.40E+04 | 7.91E+03 | 4.049E+04 | 0.872 |
| $4^3P^2(5S) 3P_1$ | $4^1P^0(5D) 3D_0$ | 36101 | 9.40E+04 | 7.91E+03 | 4.049E+04 | 0.872 |
| $4^3P^2(5S) 3P_2$ | $4^1P^0(5D) 3D_0$ | 36101 | 9.40E+04 | 7.91E+03 | 4.049E+04 | 0.872 |

Note. All transition data are in the velocity form.

(This table is available in its entirety in machine-readable form.)

Table 10

| Lower State | Upper State | $\Delta \varepsilon$ (cm$^{-1}$) | $\lambda$ (Å) | $\sigma$ | $g_f$ | $A$ (s$^{-1}$) | $dT$ |
|-------------|-------------|-------------------------------|--------------|-------|-------|---------------|------|
| $4^3P^2(5S) 3D_1$ | $4^1P^0(5D) 3P_0$ | 36101 | 9.40E+04 | 7.91E+03 | 4.049E+04 | 0.872 |
| $4^3P^2(5S) 3P_1$ | $4^1P^0(5D) 3D_0$ | 36101 | 9.40E+04 | 7.91E+03 | 4.049E+04 | 0.872 |
| $4^3P^2(5S) 3P_2$ | $4^1P^0(5D) 3D_0$ | 36101 | 9.40E+04 | 7.91E+03 | 4.049E+04 | 0.872 |

Note. All transition data are in the velocity form.

(This table is available in its entirety in machine-readable form.)

According to NIST database the fifth odd level with $J = 1/2$ is close to the fourth, meanwhile our computation shows that there is a big energy gap (12,675 cm$^{-1}$) between the fourth and fifth levels with $J = 1/2$ of 4$^f^0^6p$ configuration. Therefore, the fifth and higher levels (up to the end of the gap) can be assigned to the 4$f^5^5d^6s$ or 4$f^5^5d^2$ configurations, and this assignment is much more complicated.

The situation is similar for odd levels with $J = 3/2$ symmetry. The lowest energy levels with $J = 3/2$ for configurations 4$f^6^6p$, 4$f^5^5d^6s$, 4$f^5^5d^2$, and 4$f^7$ are at...
21,717, 24,889, 26,022, and 39,492 (in cm$^{-1}$), respectively. Therefore, the lowest energy level with $J = 3/2$ belongs to the configuration $4f^6 6p$ and the first four levels ($^6G_{3/2}, ^6D_{3/2}, ^6D_{5/2}$ and $^6G_{5/2}$) with energies 21,717, 22,283, 23,356, and 24,223 (in cm$^{-1}$) were assigned to the $4f^6 6p$ configuration (see Table 14). The sixth odd level with $J = 3/2$ can be assigned to...
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Table 13

| Lower State | Upper State | \(\Delta E\) (cm\(^{-1}\)) | \(\lambda\) (A) | \(S\) | \(gf\) | \(A\) (s\(^{-1}\)) | \(dT\) |
|-------------|-------------|----------------|----------------|------|-------|-----------------|------|
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 7731 | 12933 | 3.114E–04 | 7.313E–06 | 2.430E+01 | 0.994 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 8671 | 11531 | 1.873E–04 | 4.935E–06 | 2.063E+01 | 0.998 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 33824 | 2956 | 1.560E–06 | 1.602E–07 | 1.019E+01 | 0.031 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 34708 | 2881 | 1.269E–06 | 1.338E–07 | 8.962E+00 | 0.161 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 35251 | 2836 | 4.867E–09 | 5.212E–10 | 3.600E–02 | 0.508 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 39556 | 2528 | 5.682E–08 | 6.827E–09 | 5.938E–01 | 0.710 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 40715 | 2456 | 2.024E–08 | 2.503E–09 | 2.307E+00 | 0.669 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 41839 | 2390 | 1.941E–07 | 1.168E–07 | 1.136E+01 | 0.803 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 44260 | 2259 | 3.941E–10 | 5.299E–11 | 5.770E–03 | 0.915 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 45351 | 2196 | 7.802E–10 | 1.079E–10 | 1.243E+02 | 0.275 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 47419 | 2108 | 1.408E–07 | 2.028E–08 | 2.535E+00 | 0.426 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 49135 | 2035 | 4.078E–08 | 6.078E–09 | 8.169E–01 | 0.161 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 49860 | 2005 | 6.277E–08 | 9.508E–09 | 1.313E+00 | 0.641 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 50373 | 1985 | 5.470E–09 | 8.370E–10 | 1.180E–01 | 0.924 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 50830 | 1967 | 3.671E–09 | 5.669E–10 | 8.142E–02 | 0.933 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 52462 | 1906 | 4.967E–07 | 7.915E–08 | 1.211E+01 | 0.711 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 54181 | 1845 | 1.259E–12 | 2.072E–13 | 3.382E–05 | 0.992 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 55996 | 1785 | 2.938E–10 | 5.074E–11 | 8.844E–03 | 0.982 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 56703 | 1763 | 5.364E–09 | 9.239E–10 | 1.651E–01 | 0.920 |
| \(4f^{6}\) 6p | \(4f^{3}5d 6s\) | 57987 | 1724 | 4.101E–09 | 7.223E–10 | 1.350E–01 | 0.574 |

Note. All transition data are in the velocity form.
(This table is available in its entirety in machine-readable form.)

the \(4f^{6}\) 6p or \(4f^{3}5d 6s\) configurations, therefore we have restricted our identification of odd levels with \(J = 3/2\) up to 5 levels.

The lowest energy levels with \(J = 5/2\) for configurations \(4f^{6}\) 6p, \(4f^{3}5d 6s\), \(4f^{3}5d 2\), and \(4f^{7}\) are at 22,209; 25,250; 25,489; and 39,479 (in cm\(^{-1}\)), respectively. Therefore, the lowest energy level with \(J = 5/2\) belongs to the configuration \(4f^{6}\) 6p and the first four levels (\(5g_{5/2}, 4d_{3/2}, 4d_{5/2}, \text{ and } 4g_{3/2}\)) with energies 22,209; 22,834; 23,985; and 24,542 (in cm\(^{-1}\)) were assigned to the \(4f^{6}\) 6p configuration. The fifth level with \(J = 5/2\) can be assigned to the \(4f^{6}\) 6p or \(4f^{3}5d 6s\) configurations. Therefore, we have restricted our identification of levels with \(J = 3/2\) up to four levels.

The lowest energy levels with \(J = 7/2\) for configurations, \(4f^{6}\) 6p, \(4f^{3}5d 6s\), \(4f^{3}5d 2\), and \(4f^{7}\), are at 22,861; 20,384; 21,971; and 15,802 (in cm\(^{-1}\)), respectively. Out of four of our computed levels, three have similar energy values and are similar to the NIST energy 22,788 cm\(^{-1}\); therefore, level assignment to the configuration cannot be carried out. For the same reason, odd levels in the NIST with \(J = 7/2–15/2\) cannot be identified.

It should be noted that assignment of the configuration from NIST differs from the one computed in this study. The expansion coefficient of identified levels in this study belongs to the \(4f^{6}\) 6p configuration with at least a 0.80 value. Based on this identification, a comparison of the transition wavelength and transition probabilities with the ones obtained by Xu et al. (2003) and Lawler et al. (2006) has been done (see Figures 6 and 7).

Transition probabilities obtained in this study are found to be higher than those in Xu et al. (2003) and Lawler et al. (2006), while the transition wavelengths are in good agreement with the ones in the aforementioned studies.

4.3. Eu II

The NIST database presents 13 lines with transition probabilities that are compared with our calculations in Figure 8. There is a very good agreement of transitions probabilities, although the agreement in the transition wavelength is rather poor, about 14%.

It is worth comparing our results with more available measurements, although the data are not always critically evaluated. A summary of experiments for Eu II is given in Table 15. Absolute transitions probabilities are measured experimentally through the measurements of lifetimes (\(\tau\)) and BFs by other authors. Measurements for the lifetime are done using time-resolved laser-induced fluorescence (TR-LIF) while BFs are estimated from emission spectra of a hollow cathode discharge lamp with Eu powder in the cathode (HCL) or Fourier transform spectrometer (FTS) data. Table 15 includes the methods as well as the number of lifetimes measurements (\(N_{\tau}\)) and the number of lines (\(N_{l}\)).

Comparison with these measurement is given in Figure 9. In this figure, only the levels with clear identification are included. Most transitions are in the ranges of dashed lines showing the deviation by a factor of 2.0. However, we observe a relatively large deviation in the weak transitions: our calculations give a much smaller transition probability than those estimated from the experiments. This may suggest that our strategy of computations is not good enough for weak transitions. Another possible reason is that transitions other than E1, which we do...
Figure 4. Comparison of transition probability between the states of configurations $4f^6 6s - 4f^5 6p$ and between the states of configurations $4f^3 6p$ and $4f^4 5d$ for Pr II. The top and bottom panels show a comparison between our results and results from the NIST database. The thick line corresponds to perfect agreement, while the thin solid and dashed lines correspond to deviations by factors of 1.5 and 2.0, respectively. The black and red points show the values calculated with the length (Babushkin) and velocity (Coulomb) forms, respectively.

Figure 5. Comparison of transition wavelengths for Pr II between our results ($\lambda_{\text{cal}}$) and NIST database recommended values ($\lambda_{\text{NIST}}$). The thick line corresponds to perfect agreement, while thin solid and dashed lines correspond to 10% and 20% deviations.

Figure 6. Comparison of transition probability of Sm II between our results ($A_v$) and the results by Lawler et al. (2006) and Xu et al. (2003) ($A_{\text{exp}}$). The thick line corresponds to perfect agreement, while the thin solid and dashed lines correspond to deviations by factors of 1.5 and 2.0, respectively. Transition probabilities are presented in the velocity (Coulomb) form.

Figure 7. Comparison of transition wavelengths for Sm II between our results and experimental data by Lawler et al. (2006). The thick line corresponds to perfect agreement, while thin solid and dashed lines correspond to 10% and 20% deviations.

Table 14

| Our Label | $E_{\text{cal}}$ | NIST ILabel | $E_{\text{NIST}}$ |
|-----------|-----------------|-------------|-----------------|
| $4f^6 (^4F) 6p \ ^5G_{5/2}$ | 21418.34 | $4f^5(^7F) 6p \ ^7G$ | 21250.75 |
| $4f^6 (^4F) 6p \ ^5D_{3/2}$ | 21892.77 | $8^F$ | 21655.42 |
| $4f^6 (^4F) 6p \ ^3F_{2/1}$ | 24403.12 | $\ldots$ | 23352.41 |
| $4f^6 (^4F) 6p \ ^3F_{1/2}$ | 25378.88 | $\ldots$ | 23659.99 |
| $4f^6 (^4F) 6p \ ^3G_{3/2}$ | 21717.29 | $4f^5(^7F) 5d \ ^6s$ | 21507.87 |
| $4f^6 (^4F) 6p \ ^3D_{5/2}$ | 22283.17 | $4f^6(^7F) 6p$ | 21702.33 |
| $4f^6 (^4F) 6p \ ^3D_{3/2}$ | 23356.00 | $4f^6(^7F) 6p$ | 21904.12 |
| $4f^6 (^4F) 6p \ ^3G_{5/2}$ | 24223.90 | $4f^6(^7F) 6p$ | 23177.49 |
| $4f^6 (^4F) 6p \ ^3G_{7/2}$ | 22209.94 | $4f^5(^7F) 5d \ ^6s$ | 21813.61 |
| $4f^6 (^4F) 6p \ ^3D_{3/2}$ | 22384.78 | $4f^6(^7F) 5d \ ^6s$ | 22039.98 |
| $4f^6 (^4F) 6p \ ^3D_{3/2}$ | 23985.48 | $4f^6(^7F) 6p$ | 22248.32 |
| $4f^6 (^4F) 6p \ ^3G_{5/2}$ | 24542.98 | $4f^6(^7F) 6p$ | 22249.49 |
several experimental works to address the transition probabilities. For example, experimental transition probabilities are estimated by Corliss & Bozman (1962). Also, Wang et al. (2014) experimentally measured BFs of 12 levels for Gd II using the emission spectrum of a hollow cathode lamp. As a result, transition probabilities for 74 lines of Gd II were derived from a combination of the radiative lifetimes reported in earlier literature and newly determined BFs. Hartog et al. (2006) investigated absolute transition probabilities for 611 lines for Gd II, by using a combination of LIF radiative lifetime measurements and BF measurements. Identification of upper and lower energy levels is based on the work by Martin et al. (1978). In Figure 10, wavelengths of 460 transitions from their experiments are compared with our calculations. For comparison, we include only the levels with clear identification. Of the line wavelengths, 66% are within a 10% agreement range (solid lines) and 12% of wavelengths have more than 20% disagreement (dashed lines).

As for the transition probabilities, we obtain reasonable agreement between our computed values and the LIF measurements (Figure 11, colors of the points represent different configurations). In this figure, we include transitions with transition probabilities higher than $10^3$ from Hartog et al. (2006). Upon a closer look, however, there is disagreement, in particular for the two-electron—one-photon transitions between the states of configurations $4f^75d6p$, $4f^76s^2$, $4f^76s6p$, and $4f^75d^2$. Our calculations underestimate the experimental values of these transitions. These transitions are due to mixing of configurations in the ASFs, which allows one-electron—one-photon transitions (with one-electron jump and $\Delta l \pm 1$). The calculated values can be changed significantly by a subtle change in degrees of mixing of the allowed configurations in the ASFs. On the other hand, agreement with Hartog et al. (2006) is much better for strong transitions.

4.5. Coulomb and Babushkin Gauges for Pr II–Gd II

The wave functions are optimized on an energy expression in a variational approach. In general, this gives a better representation of the outer part of the wave functions, thus favoring the length form. The matrix element of the velocity

not include in our calculations, may contribute to these weak lines.

4.4. Gd II

For Gd II, transitions probabilities are not presented in the NIST database (Kramida et al. 2018). However, there are

| Method | MethodBF | References |
|--------|----------|------------|
| TR-LIF | HCL | Biemont et al. (1982) |
| TR-LIF | HCL | Zhang et al. (2000) |
| TR-LIF | FTS | Lawler et al. (2001) |
| TR-LIF | HCL | Wang et al. (2013) |
| TR-LIF | HCL | Tian & Wang (2019) |

Figure 8. Comparison of transition probability of Eu II between our results ($A_i$) and the NIST database. The thick line corresponds to perfect agreement, while the thin solid and dashed lines correspond to deviations by factors of 1.5 and 2.0, respectively. Transition probabilities are presented in the velocity (Coulomb) form.

Figure 9. Comparison of transition probability of Eu II between our results ($A_i$) and data of other authors ($A_{exp}$): (1) Zhang et al. (2000), (2) Komarovskii (1991), (3) Tian & Wang (2019), (4) Wang et al. (2013), (5) Lawler et al. (2001), (6) Karner et al. (1982), and Biemont et al. (1982). The thick line corresponds to perfect agreement, while the thin solid and dashed lines correspond to deviations by factors of 1.5 and 2.0, respectively. Transition probabilities are presented in the velocity (Coulomb) form.

Table 15
Summary of Experiments on Eu II

| References         | $N_f$ | Method | MethodBF |
|--------------------|-------|--------|----------|
| Biemont et al. (1982) | 27    | TR-LIF | HCL      |
| Zhang et al. (2000)  | 31    | TR-LIF | HCL      |
| Lawler et al. (2001) | 24    | TR-LIF | FTS      |
| Wang et al. (2013)   | 18    | TR-LIF | HCL      |
| Tian & Wang (2019)   | 24    | TR-LIF | HCL      |
form depends on the transition energy and it can affect the accuracy of transition probability evaluation. Because of these reasons, a much slower convergence of the velocity gauge is expected (Ynnerman & Fischer 1995). However, a paper by Papoulia et al. (2019) analyzing the convergence properties of transitions suggests that transition probabilities in the Coulomb gauge may give more accurate values. Thus, it is important to systematically study the transition data to see which gauge results in the most rapid convergence. Our comparison of forms for PrII with the NIST results shows better agreement for the velocity form.

For comparison, we computed averaged accuracy indicators of the transition probabilities, \( dT \), in the range of probability, \( \log(A_n) - \log(A_{n+1}) = 1 \). Averaged accuracy indicator values, \( dT \), for the strong transitions of all the computed ions are in Figure 12 (left y-axis). The histogram represents the numbers of transitions in the range of probability in Figure 12 (right y-axis). For example, the number of transitions is 896,662 for Pm II in the range of 5–6.

It is clearly visible that \( dT \) decreases with an increase of the transition probability, and a better agreement between the forms is expected. For Pr II–Eu II ions trends of \( dT \) are basically the same. Note that radial wave functions for Eu II were computed only for one selected \( J \) value but it unaffected by the \( dT \) trend. For Gd II, the change is visible and \( dT \) can be affected due to a different computation strategy used for Gd (see Section 2.3).

5. Summary
We presented ab initio atomic calculations of energy levels and E1 transitions from Pr II to Gd II ions based on the strategy developed for the calculations of Nd II (Gaigalas et al. 2019). In total, 2145, 9774, 8393, 2473, and 4397 levels are presented for PrII, PmII, SmII, EuII, and GdII, respectively. Some of the Rydberg states are also included to the computations for EuII. By comparing with the NIST database and the results by other authors, we confirmed that our calculations achieve good accuracy. For the energy levels, the averaged accuracy compared with the NIST data are 8%, 12%, 6%, 8%, and 7% for PrII, PmII, SmII, EuII, and GdII, respectively. These are the highest accuracies achieved for this kind of complete atomic calculations needed for opacity calculations. There is no clear dependence of accuracy on atomic number \( Z \). This means that data of lanthanide set can be computed in similar way to the isoelectronic sequence. By using the results of atomic structure calculations, E1 transitions between levels are computed. We provide data for 411,314; 7,104,005; 4,720,626; 467,724; and 1,383,694 transitions for PrII, PmII, SmII, EuII, and GdII, respectively. Transition probabilities are compared with the NIST database as well as the results of other works. Our computed E1 type transition probabilities are in good agreement with NIST database experimental values, especially in the area of strong transitions.
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