Theoretical investigation of energy levels and transition for Ce IV[★]

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ABSTRACT

Aims. We present extensive energy level and transition data for the Ce IV spectrum. By providing accurate atomic data, we evaluate the impact of atomic data on the opacity in the neutron star merger ejecta.

Methods. We performed energy spectra and transition data calculations using the GRASP2018 package, which is based on the multiconfiguration Dirac–Hartree–Fock and relativistic configuration interaction methods, and the HULLAC code, which is based on a parametric potential method.

Results. We present energy spectra calculated for the 225 levels for the Ce³⁺ ion. Energy levels are compared with recommended values from the NIST Atomic Spectra Database and other available works. The root-mean-square (rms) deviations obtained for the GRASP2018 energy levels of the 5p⁶nl configurations from the NIST data are 1270 cm^{−1}. The rms deviations for the HULLAC results from the NIST data are 5780 cm^{−1}. Furthermore, electric dipole (E1) transition data, line strengths, weighted oscillator strengths, and transition rates are computed between the above levels. The computed transition rates are compared with other theoretical computations. We also evaluate the accuracy of the wave functions and transition parameters by analyzing the dependencies of the line strength *S* on the gauge parameter *G*. The gauge dependency method also allows us to determine the transitions for which the ratio between the Babushkin and Coulomb gauges shows real agreement between forms and the transitions for which the agreement between both gauges is random. Using the GRASP2018 and HULLAC data, the opacities in the neutron star merger ejecta are also calculated. We find that the opacity of Ce IV is higher than that presented by previous works, which is because of the higher completeness of our atomic data. Although the differences in the energy levels and transition probabilities cause different features in the opacity spectrum, the *Planck* mean opacities of both data sets agree within 20%.

Key words. atomic data

1. Introduction

Observations of gravitational waves (GWs) from the neutron star (NS) merger GW170817 (Abbott et al. 2017a) and its electromagnetic counterpart (AT2017gfo, Abbott et al. 2017b) paved the way for a new method with which to study the origin of heavy elements in the Universe. The observed properties of AT2017gfo at ultraviolet, optical, and infrared wavelengths are found to be consistent with theoretically expected “kilonova”, that is, thermal emission powered by radioactive decay of newly synthesized *r*-process elements (e.g., Li & Paczyński 1998; Metzger et al. 2010). This agreement indicates that *r*-process synthesis takes place in the NS merger.

Atomic data for heavy elements can be used to interpret the observed properties of kilonovae. For example, the spectra of AT2017gfo show various broad features (e.g., Chornock et al. 2017; Pian et al. 2017; Smartt et al. 2017), which are imprints of heavy elements synthesized by the NS merger. However, the elemental species have not yet been identified, except for Sr (Watson et al. 2019; Domoto et al. 2021). To firmly identify the heavy

elements in kilonova spectra, accurate atomic data for selected, dominant transitions are necessary.

In addition, complete atomic data are also important for understanding the nucleosynthesis in the NS merger. This is because, complete atomic data are necessary to calculate the opacity in the ejecta, which in turn determines the peak luminosity and the peak timescale of the kilonova. In particular, the presence of the lanthanide elements plays an important role in shaping the light curve of a kilonova. This is because these elements have many transitions at infrared wavelengths due to the small energy spacing, which redistribute the emission from optical to near-infrared wavelengths, making the color of the kilonova redder (the physics of the formation of emission spectra of kilonovae, in particular the role of lanthanide elements, is explained in Kasen et al. 2013; Barnes & Kasen 2013; Tanaka & Hotokezaka 2013). This property was indeed used to identify GW170817/AT2017gfo as a kilonova (e.g., Chornock et al. 2017; Drout et al. 2017; Kasliwal et al. 2017; Pian et al. 2017; Smartt et al. 2017; Tanvir et al. 2017; Utsumi et al. 2017).

To better understand the link between the emission properties of a kilonova and the nucleosynthesis therein, it is important to establish the atomic opacities of heavy elements, which requires complete atomic data (i.e., energy levels up to the excited levels and transition probabilities to the excited levels). As it is difficult

[★] Table 6 is only available at the CDS via anonymous ftp to [cdsarc.u-strasbg.fr](ftp://cdsarc.u-strasbg.fr) (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/cat/J/A+A/658/A82>

to experimentally derive the complete data of energy levels and transitions, past works relied on atomic structure calculations (Kasen et al. 2013, 2017; Tanaka et al. 2018, 2020; Fontes et al. 2020; Banerjee et al. 2020). However, in such complete atomic calculations, including excited levels, the accuracy is typically low: $\sim(10\text{--}20)\%$ in the energy levels. As a result, there is a systematic uncertainty of a factor of about 2 in the opacity (Tanaka et al. 2018). To further reduce the uncertainty in the opacity, more complete and accurate atomic calculations are necessary.

In this paper, we perform *ab initio* atomic calculations for triply ionized Ce (Ce IV) and provide an extensive evaluation of the atomic data. We choose Ce^{3+} because it is one of the simplest lanthanide ions with a 4f electron in the ground configuration, and is therefore an ideal ion as a benchmark of atomic calculations for complicated lanthanide elements.

The atomic structure and transitions of Ce IV have been studied by several authors. Reader & Wyart (2009) measured the lines – most of which arise from inner-shell-excited configurations – and determined 112 energy levels. Zhang et al. (2001) measured the lifetimes for two excited levels (of the $5p^65d$ configuration) of Ce IV using the time-resolved laser-induced fluorescence technique. Savukov et al. (2003) calculated energies and transition rates for low-energy levels of Ce IV (and Pr V) using relativistic many-body perturbation theory. Safronova et al. (2015) used a configuration interaction approach with second-order perturbation theory and a linearized coupled-cluster all-order method to compute excitation energies of Ce IV along with other ions of Ce. Zilitis (2014) calculated oscillator strengths and lifetimes of the cesium isoelectronic sequence using the Dirac–Fock method. Recently, Carvajal Gallego et al. (2021) used the relativistic multiconfiguration Dirac–Hartree–Fock to compute energy spectra and radiative transition data for Ce IV, as well as Ce II and Ce III.

In the present work, we performed energy spectra computations using GRASP2018 (Froese Fischer et al. 2019) and HULLAC (Hebrew University Lawrence Livermore Atomic Code; Bar-Shalom et al. 2001) codes for the 148 energy levels of the even $5p^65d$, $5p^66s$, $5p^54f5d$, $5p^66d$, $5p^67s$, $5p^54f6s$, $5p^67d$, $5p^68s$, $5p^65g$ configurations and for the 77 levels of the odd $5p^64f$, $5p^66p$, $5p^54f^2$, $5p^65f$, $5p^67p$ configurations. Furthermore, we computed electric dipole (E1) transition data between these levels.

2. Computational procedure and scheme

2.1. GRASP2018 computations

The GRASP2018 package used for the computations is based on the multiconfiguration Dirac–Hartree–Fock (MCDHF) and relativistic configuration interaction (RCI) methods. In the MCDHF approximation, atomic state functions (ASFs) are given as linear combinations of symmetry adapted configuration state functions (CSFs),

$$\Psi(\gamma PJM) = \sum_{i=1}^{N_{\text{CSFs}}} c_i \Phi(\gamma_i PJM), \quad (1)$$

where J and M are the angular quantum numbers, P is parity, N_{CSFs} is the number of CSFs, c_i are signed amplitudes of CSF contributions, and γ contains all additional quantum numbers required to uniquely characterize a CSF. The CSFs $\Phi(\gamma_i PJM)$ are built from products of one-electron Dirac orbitals. In the relativistic self-consistent field procedure, both the radial parts of

the Dirac orbitals and the expansion coefficients were optimized to self-consistency.

In RCI computations, the atomic state function is expanded in CSFs, and only the expansion coefficients are determined by diagonalizing the Hamiltonian matrix. The RCI method was used to include the transverse-photon (Breit) interaction and the quantum electrodynamics (QED) corrections: vacuum polarization and self-energy. More details about MCHDF and RCI methods can be found in Froese Fischer et al. (2016) and Grant (2007).

In this work, ASFs were obtained as expansions over *jj*-coupled CSFs. To transform these ASFs into an *LSJ*-coupled CSF basis for labeling purposes, the method provided by Gaigalas et al. (2003, 2017) was used.

Generation of the initial wave functions begins from the MCDHF computation of the ground $[\text{Xe}]4f$ configuration. These orbitals were kept frozen and used in further computations. In the next step, the $5d$, $5f$, $5g$, $6s$, $6p$, $6d$, $7s$, $7p$, $7d$, $8s$ orbitals belonging to the configurations of the multireference (MR) set were optimized (these computations are referred to as MR below). The MR set consists of the $5p^65d$, $5p^66s$, $5p^54f5d$, $5p^66d$, $5p^67s$, $5p^54f6s$, $5p^67d$, $5p^68s$, $5p^65g$ even and $5p^64f$, $5p^66p$, $5p^54f^2$, $5p^65f$, $5p^67p$ odd configurations. A similar technique for generation of the initial wave functions was already applied to Nd ions (Gaigalas et al. 2019) and Er III (Gaigalas et al. 2020).

Unless stated otherwise, the inactive core used in the present calculations is $[\text{Kr}]4d^{10}5s^2$. The even and odd states were optimized separately. In the following steps of the MCDHF computation, active spaces (AS) of CSFs were generated by allowing single (S) substitutions from the $5p$ shell to $\{8s, 7p, 7d, 5f, 5g\}$ orbitals and single-double (SD) substitutions from the $4f$, $5d$, $5f$, $5g$, $6s$, $6p$, $6d$, $7s$, $7p$, $7d$, $8s$ shells to the orbital spaces (OS): $\text{OS}_1 = \{9s, 8p, 8d, 6f, 6g\}$, $\text{OS}_2 = \{10s, 9p, 9d, 7f, 7g, 6h\}$, and $\text{OS}_3 = \{11s, 10p, 10d, 8f, 8g, 7h\}$. Thus, valence-valence (VV) electron correlations were included in the computations. When a new OS is being computed, the previous orbitals are frozen. The MCDHF calculations were performed in the extended optimal level (EOL) scheme (Dyall et al. 1989). Table 1 summarizes the calculations performed for even and odd configurations by showing their J and parity values and the ASFs that were included in the optimization process. Based on the orbitals from the MCDHF calculations, further RCI calculations were performed, including calculation of the Breit interaction and leading QED effects. By analyzing the mean radii of the orbitals, we find that the $4f$ orbitals are closer to the other $n=4$ orbitals than either $5s$ or $5p$. Therefore, the $5s$ orbital is considered to be valence as well. Further on, the $5s$ closed shell was opened for S substitutions to the $\{8s, 7p, 7d, 5f, 5g\}$ orbitals in the RCI computations (VV2 strategy) to include additional correlation effects. In the last step, the MR set was extended to include additional important configurations based on the analysis of ASFs composition. In final computations, single-restricted-double (SrD) substitutions (allowing double (D) substitutions only from different shells) to the $\{8s, 7p, 7d, 5f, 5g\}$ orbitals were added in the active space (VV3 strategy). The inclusion of electron correlation allowing substitutions from the $5s$ shell and the extension of the MR set increase the AS very rapidly, and so limitations on substitutions were applied.

2.2. HULLAC computations

HULLAC is a coherent set of programs that calculates the atomic structure and rates of radiative and collisional processes (Bar-Shalom et al. 2001). HULLAC uses fully relativistic

Table 1. Summary of the extended optimal level MCDHF calculations performed, indicating the range of eigenvalues for each J of the even and odd configurations.

J	Parity	Eigenvalues	J	Parity	Eigenvalues
1/2	+	1–15	1/2	–	1–9
3/2	+	1–26	3/2	–	1–13
5/2	+	1–33	5/2	–	1–14
7/2	+	1–31	7/2	–	1–14
9/2	+	1–24	9/2	–	1–11
11/2	+	1–13	11/2	–	1–9
13/2	+	1–5	13/2	–	1–5
15/2	+	1	15/2	–	1–2

orbitals to calculate the energy levels and radiative transition probabilities. The atomic relativistic states are obtained from the many-electron Hamiltonian

$$H = H' + H_{\text{Breit}} + H_{\text{QED}}, \quad (2)$$

where H' is the Dirac–Coulomb Hamiltonian, and H_{Breit} and H_{QED} are the Breit interaction and QED correction used as the second-order perturbation.

The single electron orbital wavefunction is obtained by solving the Dirac equation for an effective central field potential. The effective potential is obtained by solving the Poisson equation for a nuclear point charge $Z\delta(r)$ and the electron charge distribution (Bar-Shalom et al. 2001)

$$\rho(r) = -4\pi r^2 q N [r^{l+1} \exp(-\alpha r/2)]^2, \quad (3)$$

with the boundary condition that at $r = \infty$, the potential converges to $(Z - q)/r$. Here, N is the normalization operator, q is the number of electrons, and α is the free parameter representing the average radius of the Slater type orbital. The free parameter α is obtained by minimization of the first-order configuration-average energies. For our calculation of Ce IV, the central potential as seen by the last electron is determined by removing one electron from the ground configuration $5p^6 4f$ (Kramida et al. 2020), which gives $5p^6$. The potential is also optimized for the ground configuration. We note that the energy levels for Ce IV are calculated for all the configurations of the MR set mentioned in Sect. 2.1, including the ground state.

The N -electron zero-order solution or the configuration state function (CSF) are derived as the anti-symmetrized product of the single-electron zero-order solution of the orbitals in the chosen coupling scheme (jj in this case). A Hamiltonian matrix, including the Breit interaction and the leading QED correction of multi-CSFs, is diagonalized as in the RCI method of GRASP2018. As a result, ASFs are obtained as linear combinations of the CSFs.

3. Results

3.1. Evaluation of energy spectra

In this work, excitation energies were computed for the 148 states of the even $5p^6 5d$, $5p^6 6s$, $5p^5 4f 5d$, $5p^6 6d$, $5p^6 7s$, $5p^5 4f 6s$, $5p^6 7d$, $5p^6 8s$, and $5p^6 5g$ configurations and for the 77 states of the odd $5p^6 4f$, $5p^6 6p$, $5p^5 4f^2$, $5p^6 5f$, and $5p^6 7p$ configurations using the GRASP2018 and HULLAC codes. Table A.1 displays

energy spectra and the atomic state function composition in LS -coupling from the GRASP2018 calculations for levels of these configurations. The levels are given with unique labels (Gaigalas et al. 2017). In the computed spectra there are levels, for which the assigned labels are not based on the largest contribution to the composition. These are marked in bold font in Table A.1. Energy levels were computed up to the 31 eV energy limit.

The Atomic Spectra Database (ASD) of the National Institute of Standards and Technology (NIST; Kramida et al. 2020) provides only 16 energy levels of the $5p^6 nl$ configurations for the Ce IV spectrum; these are based on Lang (1936). Reader & Wyart (2009) presented 112 experimental energy levels, most of them belonging to the inner-shell-excited configurations ($5p^5 4f 5d$ and $5p^5 4f 6s$). Energy levels given by Reader & Wyart (2009) fully agree with the values given in the NIST ASD (Kramida et al. 2020) except energies for the $5p^6 7d \ ^2D_{5/2}$ and $5p^6 5g \ ^2G_{7/2,9/2}$ states. Reader & Wyart (2009) found the Lang (1936) $5g$, $7d_{5/2}$, and $8s$ levels to be spurious and determined new values for the $5p^6 7d \ ^2D_{5/2}$ state and for the states of the $5p^6 5g$ configuration.

To evaluate the accuracy of the results, the calculated energy levels were compared with data from the NIST ASD (Kramida et al. 2020) and experimental or other theoretical results. The comparison of computed (with GRASP2018 and HULLAC codes) energy levels and experimental (Reader & Wyart 2009) or theoretical ones (Savukov et al. 2003 and Safronova et al. 2015) with the NIST ASD, giving a difference (in cm^{-1}) $\Delta E = E_{\text{NIST}} - E_{\text{calc}}$, is presented in Table 2. The NIST ASD specifies one energy value ($225\,625 \text{ cm}^{-1}$) for the two unresolved levels of the $5p^6 5g$ configuration. When comparing this energy level with other works, the level with the lower energy was compared. In the case of Reader & Wyart (2009) and GRASP2018 results, the lower energy belongs to the level with $J = 7/2$, while in the case of HULLAC, the lower level has $J = 9/2$. As we can see from the table, computed energies of GRASP2018 agree well with recommended values from the NIST ASD. The root-mean-square (rms) deviations obtained for energy levels of the $5p^6 nl$ configurations from the NIST data are 1270 cm^{-1} . The HULLAC energy levels in comparison with the NIST data are too high, and the rms deviations from the NIST data are 5780 cm^{-1} . When comparing the results of other theoretical investigations (Savukov et al. 2003 and Safronova et al. 2015) with the NIST ASD, the rms deviations are 2160 cm^{-1} and 2240 cm^{-1} , respectively; but those authors only investigated low-lying levels.

It should be mentioned that the order of the levels of the $5p^6 6d \ ^2D$ term in the GRASP2018 results disagrees with the NIST ASD. Considering the order of these states in HULLAC studies and in the calculations performed by Savukov et al. (2003), it is seen that the order agrees with the NIST ASD, but the splitting is much smaller. In the HULLAC case, it is only 15 cm^{-1} , in Savukov et al. (2003) it is 720 cm^{-1} , while in the NIST ASD this splitting reaches 1715 cm^{-1} . Reader & Wyart (2009) show that this anomalous fine structure is the result of interaction between $5p^6 6d$ and the inner-shell excited configuration $5p^5 4f 5d$. Whereas there is good agreement between GRASP2018 and NIST data for most energy levels, and the order for other levels is correct, a deeper analysis was performed for the levels of the $5p^6 6d \ ^2D$ term to clarify this disagreement. In Fig. 1, the convergence of these levels by including different correlations is presented. As seen from the figure, in the MR computations, the $5p^6 6d \ ^2D_{3/2}$ level is lower than $5p^6 6d \ ^2D_{5/2}$. By including the correlations (VV2), the order of the levels is inverted and does not change by extending the orbital space. It

Table 2. Comparison of energy levels from the present work and other experimental or theoretical studies with the NIST ASD (deviations in cm^{-1}) for Ce IV.

Config.	Term	J	NIST	1	GRASP2018	HULLAC	2	3
$5p^6 4f$	$^2F^o$	7/2	2253	2252.50	2053/ 200	2081/ 172	2214/ 39	2187/ 66
$5p^6 5d$	^2D	3/2	49 737	49 737.30	47 653/2084	50 098/ -361	47 563/ 2174	47 535/2202
$5p^6 5d$	^2D	5/2	52 226	52 226.33	50 163/2063	52 526/ -300	50 146/2080	49 966/2260
$5p^6 6s$	^2S	1/2	86 602	86 602.10	86 031/ 571	93 253/-6651	84 578/2024	84 006/2596
$5p^6 6p$	$^2P^o$	1/2	122 585	122 585.29	121 809/ 776	129 246/-6661	120 481/2104	120 014/2571
$5p^6 6p$	$^2P^o$	3/2	127 292	127 292.24	126 396/ 896	133 570/-6278	125 136/2156	124 701/2591
$5p^6 6d$	^2D	5/2	177 198	177 199.23	176 236/ 962	183 448/-6250	175 072/2126	
$5p^6 6d$	^2D	3/2	178 913	178 913.57	175 495/3418	183 463/-4550	175 792/3121	
$5p^6 7s$	^2S	1/2	183 502	183 501.73	182 938/ 564	188 579/-5077	181 176/2326	
$5p^6 5f$	$^2F^o$	5/2	184 545	184 543.00	183 913/ 632	192 660/-8115		
$5p^6 5f$	$^2F^o$	7/2	184 746	184 744.88	184 167/ 579	192 631/-7885		
$5p^6 7d$	^2D	3/2	221 661	221 661.70	221 463/ 198	228 226/-6565		
$5p^6 7d$	^2D	5/2	221 838	222 579.25	221 952/-114	228 620/-6782		
$5p^6 8s$	^2S	1/2	225 128		225 137/ -9	231 118/-5990		
$5p^6 5g$	^2G	7/2,9/2	225 625	226 771.66	225 466/ 159	231 349/-5724		

References. (1) Reader & Wyart (2009); (2) Savukov et al. (2003); (3) Safronova et al. (2015).

Fig. 1. Convergence of the $5p^6 6d \ ^2D_{3/2}$ and $5p^6 6d \ ^2D_{5/2}$ levels when different electron correlation effects are included. OS₁–OS₃ marks the results from the VV2 strategy, OS₃* marks the results from the VV3 strategy.

was shown that the energy values converge to the NIST results by extending the orbital space from OS₁ to OS₃ (in the VV2 strategy), and the energies are very close to the NIST recommended values at OS₃. By including the additional correlations (VV3 strategy; see OS₃* in Fig. 1), the order of the states is inverted and the $^2D_{3/2}$ level becomes the lower one. The figure also shows that the Breit and QED corrections have little influence on the energies. In Fig. 1, HULLAC results are also presented. HULLAC energy levels can be seen to be higher than energies given in the NIST ASD, and as the splitting between the fine-structure levels is very small, results for the two levels overlap.

We also analyzed the composition of these levels present our findings in Fig. 2 and Table 3. In Fig. 2 only the main contributors from different strategies are presented, while Table 3 shows the total contribution of each configuration to these two levels when different strategies are applied. After including correlations with the VV3 strategy, the weight of the $5p^6 6d$

Fig. 2. Fractional coefficients of the main contributors to the $5p^6 6d \ ^2D_{3/2}$ and $5p^6 6d \ ^2D_{5/2}$ levels including different electron correlation effects. OS₁–OS₃ marks the results from the VV2 strategy, OS₃* marks the results from the VV3 strategy.

configuration decreases in the $5p^6 6d \ ^2D_{3/2}$ level, and the influence of the $5p^5 4f 5d$ configuration increases. For the $5p^6 6d \ ^2D_{5/2}$ state, the situation is vice versa. From Fig. 2 it is seen that the $5p^6 6d \ ^2D_{3/2}$ state is quite pure in the HULLAC computations (about 88%), while in the final GRASP2018 results the $5p^6 6d$ contribution is smaller; it constitutes 58% in the composition and is close to that found by Reader & Wyart (2009). The $5p^6 6d \ ^2D_{5/2}$ state is purer (about 80%) in the final GRASP2018 calculations, while in the HULLAC and Reader & Wyart (2009) investigations, it is 48% and 50%, respectively. From the analysis, it is seen that the change in the order of the two states in the final results is affected by the MR set extension and inclusion of additional correlations in the VV3 strategy. To study the accuracy of the GRASP2018 results, we also analyzed the convergence for the levels with the same orbital angular momenta ($l = 3$) but with higher principal quantum number ($n = 7$). Figure 3 presents the convergence of the $5p^6 7d \ ^2D$ term states

Fig. 3. Convergence of the $5p^6 7d \ ^2D_{3/2}$ and $5p^6 7d \ ^2D_{5/2}$ levels when different electron correlation effects are included. OS₁–OS₃ marks the results from the VV2 strategy, OS₃* marks the results from the VV3 strategy.

Fig. 4. Differences between experimental energy levels of Reader & Wyart (2009) and those of the present GRASP2018 calculations (in cm⁻¹). “HE” means levels with the highest calculated energies (>230 000 cm⁻¹). All HE levels belong to the $5p^5 4f 5d$ configuration.

when different correlations are included. Energy levels of the $5p^6 7d$ configuration in the final results agree very well with NIST data. The fine-structure levels of the $5p^6 7d \ ^2D$ term have the same trends as those of the $5p^6 6d \ ^2D$ term. The $^2D_{3/2}$ and $^2D_{5/2}$ levels are inverted when the VV2 strategy is used, and the order of the states changes when correlations are added with the VV3 strategy. The accuracy of the results and the quality of the wave functions of the $5p^6 6d \ ^2D$ term are analyzed in Sect. 3.2.

Figures 4 and 5 present the comparison of computed (with the GRASP2018 and HULLAC codes) energy levels with energy levels given by Reader & Wyart (2009). The HULLAC and GRASP2018 energy levels were related by comparing the compositions in jj coupling with the data of Reader & Wyart (2009). Figures 4 and 5 show three distinct groups of energy levels. As seen from Fig. 4, the agreement with GRASP2018 for the levels of the $5p^5 4f nl$ configurations is poorer than it is for the $5p^6 nl$ configurations, the difference reaches 16 000 cm⁻¹ for some levels. The HULLAC results (see Fig. 5) are in good agreement with those of Reader & Wyart (2009) for the levels of the $5p^5 4f 5d$ and $5p^5 4f 6s$ configurations. The rms deviations for energy spectra of

Fig. 5. Differences between experimental energy levels of Reader & Wyart (2009) and those of the present HULLAC calculations (in cm⁻¹). “HE” means levels with the highest calculated energies (>230 000 cm⁻¹). All HE levels belong to the $5p^5 4f 5d$ configuration.

these configurations from the Reader & Wyart (2009) data are displayed in Table 4.

3.2. Evaluation of transition data

The accuracy of the wave functions and the uncertainties of the transition parameters were evaluated by: (1) analyzing the dependence of the line strength S on the gauge parameter G (Rudzikas 2007); (2) analyzing the dependence of the cancellation factor (CF; Cowan 1981) on the gauge parameter G ; (3) studying the dT parameter defined in Ekman et al. (2014), which shows the relative difference between the Babushkin and Coulomb gauges of the computed transition rates; (4) comparing the computed transition data with other available data. For this purpose transitions from different regions of energy spectra were chosen as illustrated in Fig. 6. Firstly, the accuracy of the wave functions was evaluated by studying the transition parameters as a function of G .

The dependence of the line strength S on G is parabolic,

$$S(G) = aG^2 + bG + c, \quad (4)$$

where

$$a = \frac{A}{2}(M_B - M_C)^2, \quad (5)$$

$$b = A\sqrt{2}M_C(M_B - M_C), \quad (6)$$

$$c = AM_C^2. \quad (7)$$

A is a coefficient, and in the case where $S(G)$ represents the line strength, is expressed as

$$A = \frac{c^2(2J_{\text{lower}} + 1)}{2\Delta E^2}, \quad (8)$$

where c is the speed of light and ΔE is transition energy. M_B and M_C are the reduced matrix elements $\langle \Phi(\gamma_j P J) \| \mathbf{T}^{(1)} \| \Phi(\gamma_k' P' J') \rangle$ (see Eq. (3) in Gaigalas et al. 2020) in the Babushkin ($G = \sqrt{2}$) and Coulomb ($G = 0$) gauges, respectively. Generally, the quadratic equation has two roots. Equation (4) with the coefficients a , b , and c given by Eqs. (5), (6), and (7), has only one

Table 3. Composition (with sum contributors of the configuration $> 0.5\%$) for the $5p^6 6d^2 D_{3/2}$ and $5p^6 6d^2 D_{5/2}$ levels from different strategies.

Strategy	Composition
$5p^6 6d^2 D_{3/2}$ level	
MR	$34.75 5s^2 5p^6 6d + 64.75 4f 5s^2 5p^5 5d$
VV2 OS ₁	$71.47 5s^2 5p^6 6d + 24.08 4f 5s^2 5p^5 5d + 1.33 5s^2 5p^5 6p 6d$
VV2 OS ₂	$73.06 5s^2 5p^6 6d + 22.48 4f 5s^2 5p^5 5d + 1.35 5s^2 5p^5 6p 6d + 0.50 5s^2 5p^5 6d 8p$
VV2 OS ₃	$72.97 5s^2 5p^6 6d + 22.57 4f 5s^2 5p^5 5d + 1.35 5s^2 5p^5 6p 6d + 0.50 5s^2 5p^5 6d 8p$
VV3 OS ₃	$57.72 5s^2 5p^6 6d + 36.17 4f 5s^2 5p^5 5d + 1.07 5s^2 5p^4 5d^2 6d + 0.91 5s^2 5p^5 6p 6d$
$5p^6 6d^2 D_{5/2}$ level	
MR	$74.09 5s^2 5p^6 6d + 25.37 4f 5s^2 5p^5 5d$
VV2 OS ₁	$63.21 5s^2 5p^6 6d + 32.21 4f 5s^2 5p^5 5d + 1.17 5s^2 5p^5 6p 6d$
VV2 OS ₂	$63.39 5s^2 5p^6 6d + 31.954 f 5s^2 5p^5 5d + 1.18 5s^2 5p^5 6p 6d$
VV2 OS ₃	$63.62 5s^2 5p^6 6d + 31.724 f 5s^2 5p^5 5d + 1.18 5s^2 5p^5 6p 6d$
VV3 OS ₃	$80.29 5s^2 5p^6 6d + 12.624 f 5s^2 5p^5 5d + 1.48 5s^2 5p^4 5d^2 6d + 1.28 5s^2 5p^5 6p 6d + 0.53 4f^2 5s^2 5p^4 6d$

Table 4. rms deviations of energy spectra (in cm^{-1}) for the different groups of the configurations from GRASP2018 and HULLAC results.

Configuration	GRASP2018	HULLAC
$5p^6 nl$	1413	5517
$5p^5 4f nl$	13 980	2542
HE	23 800	22461

Notes. Differences are computed comparing with Reader & Wyart (2009) results. “HE” means levels with the highest calculated energies ($> 230\,000 \text{ cm}^{-1}$). All HE levels belong to the $5p^5 4f 5d$ configuration.

Fig. 6. Scheme of transitions that were investigated to evaluate the accuracy of the wave functions and transition parameters. The numbering and labeling of the levels match Table A.1.

root given by Eq. (9). The more accurate the wave functions, the flatter (the smaller the a and the larger the G value for which $S = 0$ ($G_{S=0}$)) the gauge dependence of the line strengths (Rudzikas 2007; Gaigalas et al. 2010). The a value is smaller when the agreement between the reduced transition matrix elements of the two gauges is better. The minimum of the parabola is defined as

$$G_{S=0} = \frac{\sqrt{2}M_C}{M_C - M_B}, \quad (9)$$

and is larger when the difference between the matrix elements of the two gauges is smaller. In the case where matrix elements fully agree in both gauges, the transition parameter is independent of G .

Fig. 7. Gauge dependence of the $5s^2 5p^6 6p^2 P_{1/2} - 5s^2 5p^6 5d^2 D_{3/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class A.

$G_{S=0}$ parameter can be expressed through the line strength:

$$G_{S=0} = \frac{\text{sgn}(M_C) \sqrt{2S_C}}{\text{sgn}(M_C) \sqrt{S_C} - \text{sgn}(M_B) \sqrt{S_B}}, \quad (10)$$

where $\text{sgn}(M_B) = \frac{M_B}{|M_B|}$ and $\text{sgn}(M_C) = \frac{M_C}{|M_C|}$ shows the sign of reduced transition matrix elements in the Babushkin and Coulomb gauges, respectively. S_B and S_C are the line strengths in the Babushkin and Coulomb gauges, respectively. When the $G_{S=0}$ parameter is expressed through the line strength, the sign of the reduced transition matrix element is very important. In the range $-\infty < G_{S=0} < 0$ and $\sqrt{2} < G_{S=0} < \infty$, matrix elements usually have the same sign in the two forms. When $0 < G_{S=0} < \sqrt{2}$, the matrix elements are of different sign in the two forms.

The minimum of the parabola is related to the dT parameter by the expression

$$|G_{S=0}| = \left| \frac{\sqrt{2S_C}(\text{sgn}(M_C) \sqrt{S_C} + \text{sgn}(M_B) \sqrt{S_B})}{dT \times \max(S_C, S_B)} \right|. \quad (11)$$

The dependencies of the line strengths on the gauge parameter G for the studied transitions are displayed in Figs. 7–13.

Fig. 8. Gauge dependence of the $5s^2 5p^6 5d \ ^2D_{3/2} - 4f 5s^2 5p^6 \ ^2F^\circ_{5/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class D+.

Fig. 11. Gauge dependence of the $4f 5s^2 5p^5 ({}^3F) 5d \ ^2F_{7/2} - 4f 5s^2 5p^6 \ ^2F^\circ_{7/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class D+.

Fig. 9. Gauge dependence of the $5s^2 5p^6 5g \ ^2G_{9/2} - 5s^2 5p^6 5f \ ^2F^\circ_{7/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class B.

Fig. 12. Gauge dependence of the $5s^2 5p^6 6d \ ^2D_{3/2} - 5s^2 5p^6 6p \ ^2P^\circ_{3/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class A.

Fig. 10. Gauge dependence of the $4f 5s^2 5p^5 ({}^3D) 5d \ ^2F_{5/2} - 4f 5s^2 5p^6 \ ^2F^\circ_{5/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class B.

Fig. 13. Gauge dependence of the $5s^2 5p^6 5f \ ^2F^\circ_{5/2} - 5s^2 5p^6 6d \ ^2D_{5/2}$ E1 line strength for the Ce^{3+} ion. The dashed lines mark the values of the line strength from other works. This transition is assigned to the accuracy class B+.

Table 5. $G_{S=0}$ and dT values for the studied transitions of the final results (the VV3 strategy).

Transition	$G_{S=0}$	dT
$5s^2 5p^6 6p \ ^2P_{1/2}^\circ - 5s^2 5p^6 5d \ ^2D_{3/2}$	123.006	0.02286
$5s^2 5p^6 5d \ ^2D_{3/2} - 4f 5s^2 5p^6 \ ^2F_{5/2}^\circ$	11.816	0.22504
$5s^2 5p^6 5g \ ^2G_{9/2} - 5s^2 5p^6 5f \ ^2F_{7/2}^\circ$	-35.305	0.07554
$4f 5s^2 5p^5(^3D) 5d \ ^2F_{5/2} - 4f 5s^2 5p^6 \ ^2F_{5/2}^\circ$	-30.131	0.08765
$4f 5s^2 5p^5(^3F) 5d \ ^2F_{7/2} - 4f 5s^2 5p^6 \ ^2F_{7/2}^\circ$	-9.9750	0.23292
$5s^2 5p^6 6d \ ^2D_{3/2} - 5s^2 5p^6 6p \ ^2P_{3/2}^\circ$	109.920	0.02557
$5s^2 5p^6 5f \ ^2F_{5/2}^\circ - 5s^2 5p^6 6d \ ^2D_{5/2}$	64.086	0.04365

Here, the lines strengths from the present HULLAC computations and from other works are also plotted. As seen from the figures, the correlations included in the final computations (the VV3 strategy) are very important for all studied transitions and especially for transitions between highly excited levels or from highly excited levels to the ground configuration (Figs. 9–13). In Figs. 7–8, the gauge dependence changes monotonically upon increasing the orbital spaces or upon including additional correlations. For the studied transitions, the dependence is closer to linear when correlations included in the final computations (the VV3 strategy) are added. Also, the minimum position of the parabola (the $G_{S=0}$ values) – which shows the accuracy of the wave functions – for the VV3 strategy is larger than for other strategies. Thus, the wave functions of the final results should be more accurate than from the VV2 strategy. The dT parameter for the studied transitions was poorer for all choices of OS of the VV2 strategy than in the final results. The $G_{S=0}$ values together with the dT parameters of the VV3 strategy are presented in Table 5. The magnitude of dT is smaller for transitions that have more accurate wave functions. The minimum position of the parabola is also important for predicting how the results will change by improving the calculations. If the Babushkin and Coulomb gauges are close to the minimum position of the parabola, then improving the computations will not significantly change the results. If the Babushkin and Coulomb gauges are on the parabola, then improvement of the computations will lead to a relatively large change in the results.

In this section, we present the results of an evaluation of the quality of the wave functions for the $5p^6 6d \ ^2D_{3/2}$ and $5p^6 6d \ ^2D_{5/2}$ levels which was carried out because a disagreement was found in the order of these levels as compared with the NIST data. To this end, we analyzed the transitions in which the $5p^6 6d \ ^2D$ term participates, and the dependence of the line strength S on the gauge parameter G is presented in Figs. 12–13. By analyzing the gauge dependence, we see that the wave functions of the $5p^6 6d \ ^2D$ levels in the final computations (the VV3 strategy) are more accurate than they are in other strategies. From the analysis, it follows that the final results (the VV3 strategy, with the $5p^6 6d \ ^2D_{3/2}$ level lower than $5p^6 6d \ ^2D_{5/2}$) are more accurate than results from other strategies.

Further, to determine which gauge parameter G is more suitable, we studied the cancellation factor (CF; Cowan 1981). The dependencies of the CF on the gauge parameter G for the studied transitions are shown in Figs. 14–20. A small value of the CF, for example less than 0.1 or 0.05 (these values are given in Cowan (1981)), indicates that the calculated transition parameter is affected by strong cancellation effects. By analyzing these transitions, it was observed that transition data in the Babushkin

Fig. 14. Dependence of the cancellation factor on gauge for the $5s^2 5p^6 6p \ ^2P_{1/2}^\circ - 5s^2 5p^6 5d \ ^2D_{3/2}$ transition for the Ce^{3+} ion. **Fig. 15.** Dependence of the cancellation factor on gauge for the $5s^2 5p^6 5d \ ^2D_{3/2} - 4f 5s^2 5p^6 \ ^2F_{5/2}^\circ$ transition for the Ce^{3+} ion. **Fig. 16.** Dependence of the cancellation factor on gauge for the $5s^2 5p^6 5g \ ^2G_{9/2} - 5s^2 5p^6 5f \ ^2F_{7/2}^\circ$ transition for the Ce^{3+} ion.

gauge are less affected by cancellation effects than transition data in other gauges, except the gauge with $G=1$, which gives even larger CFs than the Babushkin gauge in the $5s^2 5p^6 6p \ ^2P_{1/2}^\circ - 5s^2 5p^6 5d \ ^2D_{3/2}$, $4f 5s^2 5p^5(^3D) 5d \ ^2F_{5/2} - 4f 5s^2 5p^6 \ ^2F_{5/2}^\circ$, and

Fig. 17. Dependence of the cancellation factor on gauge for the $4f 5s^2 5p^5(^3D) 5d ^2F_{5/2}-4f 5s^2 5p^6 ^2F_{5/2}$ transition for the Ce^{3+} ion.

Fig. 19. Dependence of the cancellation factor on gauge for the $5s^2 5p^6 6d ^2D_{3/2}-5s^2 5p^6 6p ^2P_{3/2}$ transition for the Ce^{3+} ion.

Fig. 18. Dependence of the cancellation factor on gauge for the $4f 5s^2 5p^5(^3F) 5d ^2F_{7/2}-4f 5s^2 5p^6 ^2F_{7/2}$ transition for the Ce^{3+} ion.

Fig. 20. Dependence of the cancellation factor on gauge for the $5s^2 5p^6 5f ^2F_{5/2}-5s^2 5p^6 6d ^2D_{5/2}$ transition for the Ce^{3+} ion.

$4f 5s^2 5p^5(^3F) 5d ^2F_{7/2}-4f 5s^2 5p^6 ^2F_{7/2}$ transitions. By analyzing the dependence of the CF on the gauge parameter G , it is seen that the trend of the dependence for the studied transitions is similar, the peak (the largest value of the CF) in all strategies is for $G = 1$ or $G = \sqrt{2}$, except the $4f 5s^2 5p^5(^3D) 5d ^2F_{5/2}-4f 5s^2 5p^6 ^2F_{5/2}$ transition (see Fig. 17). For this transition, CFs with $G > 1$ are larger in the OS_1-OS_3 spaces using the VV2 strategy. The situation changes when the VV3 are included in the computations. Based on this analysis, the transition parameters were computed in the Babushkin gauge.

Table A.2 presents a comparison of the computed wavelengths and transition probabilities with results from Reader & Wyart (2009), Carvajal Gallego et al. (2021), and Savukov et al. (2003). The rms of the relative differences of the GRASP2018 results from the experimental wavelengths (Reader & Wyart 2009) is about 2%, 11%, and 19% for transitions between $5p^6nl - 5p^6nl$, $5p^6nl - 5p^54fnl$, and $5p^6nl-HE$, respectively. Carvajal Gallego et al. (2021) presented transition rates for 37 lines of Ce IV. However, these authors do not give the energy spectra in their paper for this ion. Therefore, only transitions for which the energy levels could be related with the NIST energies have been compared here.

Fig. 21. Comparison of computed line strengths of E1 transitions in Ce IV with results from Reader & Wyart (2009), Carvajal Gallego et al. (2021), and Savukov et al. (2003).

Figure 21 presents a comparison of the computed line strengths from the present work and other theoretical calculations (Carvajal Gallego et al. 2021; Savukov et al. 2003) with results from Reader & Wyart (2009). The agreement between all theoretical methods is similar, except for three transitions from

Fig. 22. Comparison of the computed line strengths of E1 transitions in Ce IV with results from Reader & Wyart (2009). Transitions between different groups of the configurations are distinguished.

Fig. 23. Comparison of the computed line strengths of E1 transitions in Ce IV from different strategies of the GRASP2018 with results from Reader & Wyart (2009).

$5p^65d$ to the ground configuration, for which all other calculations do not agree with the results from Savukov et al. (2003). The best agreement with results from Reader & Wyart (2009) was achieved for transitions (with $S > 1$), where the rms deviations for all theoretical methods are about (11–15)%. It should be mentioned that all transitions presented in Fig. 21 are between levels of the $5p^6nl$ configurations. Figure 22 presents a comparison of the computed line strengths from GRASP2018 with results of Reader & Wyart (2009), where transitions between different groups of configurations are distinguished. The agreement between both results and the deviations within the same line strength range differ for transitions from different groups. This is especially notable for transitions with greater line strength. Figure 23 presents a comparison of transitions of the $5p^6nl$ group between the results from two GRASP2018 strategies and the results from Reader & Wyart (2009). Here, most of the results are in better agreement with the VV2 strategy, which by the analysis presented above was evaluated as less accurate than the VV3 strategy.

Usually, calculated transition rates are more accurate for greater line strengths than for weaker ones. By analyzing the agreement of the line strength of the final GRASP2018 results between both forms, it was observed that ratios of the two

Fig. 24. Comparison of the computed line strengths of E1 transitions between the Babushkin and Coulomb forms in Ce IV (the VV3 strategy, the final GRASP2018 results). Transitions between different groups of the configurations are distinguished.

Fig. 25. Distribution of line strength S as a function of the $G_{S=0}$ parameter.

forms have different distributions within the same range of line strengths, depending on the configurations involved. Some of the computed GRASP2018 transitions are presented in Fig. 24, where transitions between different groups of configurations are distinguished. Deviations of line strengths for the transitions from different groups differ within the same line strength range. This is also seen in Fig. 22, where the results from the present study are compared with those of Reader & Wyart (2009). This means that not all levels are described with equal accuracy, even levels from the same configuration group. When a large number of levels is computed, and the highest levels are close to the ionization limit, it is quite difficult to achieve the same accuracy for all computed levels. The goal of this work is to compute as many levels as possible, taking into account the complexity of the task and limitation of computer resources. Therefore, 225 energy levels were computed up to the 31 eV energy limit, which is close to the ionization energy (36.906 eV). Also, all possible transitions were calculated between these levels. From the above analysis, it follows that the accuracy of the transitions with similar line strengths should likely be different. Here, transitions were plotted against the $G_{S=0}$ parameter, which helps to identify the most accurate transitions.

The distribution of line strength S as a function of $G_{S=0}$ parameter is presented in Fig. 25. From the gauge

Fig. 26. Natural logarithm of the ratio of the line strength S in the Babushkin form to the line strength S in the Coulomb form, as a function of the $G_{S=0}$ parameter. The figures show the results of present transition calculations (each dot represents a certain transition). Panel (a) shows three distinct parts, each plotted on a separate graph: (1) the upper part of the graph (blue points), where $-\infty < G_{S=0} < 0$ (or part b); (2) the lower left part of the graph (red points), where $0 < G_{S=0} < \sqrt{2}$ (or part c); and (3) the lower right part of the graph (green points), where $\sqrt{2} < G_{S=0} < \infty$ (or part d).

dependence analysis, which shows the quality of the wave functions (Rudzikas 2007), it follows that the most accurate results have greater $G_{S=0}$. Figure 25 shows that the most accurate results are in different ranges of line strengths. For example, if the $G_{S=0}$ parameter is fixed at a value of 100, the values of the line strength S vary in the range of (0.0001–20) a.u. Also, the line strengths of similar magnitude have different accuracy. For example, if the range of $S = (0.01\text{--}0.1)$ a.u. is fixed, the $G_{S=0}$ parameter varies in the range (0.01–6000). Therefore, if transitions with similar line strengths are evaluated together, the accuracy will be overestimated or underestimated for some of them, depending on the $G_{S=0}$ parameter.

Taking all of the above into account, the uncertainties of the final GRASP2018 transition data were estimated based on quantitative and qualitative evaluation of the transition parameters. Figure 26 shows the connection between quantitative (natural logarithm of the ratio of line strength S in the Babushkin form to the line strength S in the Coulomb form) and qualitative (gauge dependence analysis) evaluation of the transition data. Figure 26 can be divided into three parts: (1) the upper part of the graph (blue points), where $-\infty < G_{S=0} < 0$; (2) the lower left part of the graph (red points), where $0 < G_{S=0} < \sqrt{2}$; and (3) the lower right part of the graph (green points), where $\sqrt{2} < G_{S=0} < \infty$. In the case where $G_{S=0}$ is in the range between the Coulomb and Babushkin gauges (the lower left part of Fig. 26), the values of the transition parameter in

the two forms are on different branches of the parabola represented by Eq. (4). In this case, the agreement between both gauges is random, and cannot be used as the accuracy indicator. In two other cases, when the value of $G_{S=0}$ is smaller than zero or greater than $\sqrt{2}$, the values in the Coulomb and Babushkin gauges are on the same branch of the parabola of Eq. (4), the ratio between the two shows real agreement and can be used for accuracy estimation. Therefore, only transitions belonging to the ranges with $-\infty < G_{S=0} < 0$ or $\sqrt{2} < G_{S=0} < \infty$ can be evaluated based on the ratio between the two gauges. The computed transition strengths from these two groups were divided into groups according to the natural logarithm of the ratio (see Fig. 27). Transitions with similar agreement between the two gauges (or with similar $G_{S=0}$ parameter) were assigned to the same accuracy class. The limits of the accuracy classes were chosen according to the NIST ASD (Kramida et al. 2020) terminology (AA $\leq 1\%$, A+ $\leq 2\%$, A $\leq 3\%$, B+ $\leq 7\%$, B $\leq 10\%$, C+ $\leq 18\%$, C $\leq 25\%$, D+ $\leq 40\%$, D $\leq 50\%$, and E $> 50\%$). All the remaining transitions with $0 < G_{S=0} < \sqrt{2}$ were not evaluated, and were assigned to the accuracy class E.

To evaluate the total uncertainties of A and gf values, the uncertainties of the transition energy should be added. Transition energy uncertainties should be scaled by a factor of 3 for A or by factor of 1 for gf , because A is proportional to the cube of transition energy ΔE , while gf is proportional to the first power of ΔE .

Table 7. Comparison of the computed lifetimes (in ns) for Ce IV with experimental results and other theoretical calculations.

State	This work			Exp. 3	Th.			
	1	1(adj.)	2		3	4	5	6
$5p^6 5d \ ^2D_{3/2}$	24.61	21.65(29.0)	19.98	$30(1^\beta + 1^\theta)$	30.5	29.3	11.68	
$5p^6 5d \ ^2D_{5/2}$	22.98	20.49(28.5)	18.92	$30(1.4^\beta + 1.6^\theta)$	30.0	28.3	11.28	
$5p^6 6p \ ^2P_{1/2}^\circ$	0.69	0.72(3.1)	0.55			0.73	0.72	0.614
$5p^6 6p \ ^2P_{3/2}^\circ$	0.61	0.63(3.2)	0.52			0.62	0.63	0.506

Notes. Lifetimes of GRASP2018 calculations are given in the Babushkin form. Lifetimes in the ‘1(adj.)’ column were recalculated using the experimental wavelengths for the radiative transition probabilities. The estimated uncertainty on the lifetime was calculated using the relative difference (in %) $(\tau_B - \tau_C)/\min(\tau_B, \tau_C)$ and is given in parentheses.

References. (1) GRASP2018 results; (2) HULLAC results; (3) Zhang et al. (2001) (β : statistical error; θ : estimated systematic error); (4) Reader & Wyart (2009); (5) Savukov et al. (2003); (6) Zilitis (2014) (lifetimes are given in the Babushkin form).

Fig. 27. Natural logarithm of the ratio of the line strength S in the Babushkin form to the line strength S in the Coulomb form, as a function of the $G_{S=0}$ parameter in the range where $\ln(S_B/S_C)$ reflects the real accuracy of the calculation (right part of Fig. 26 a). The limits of the accuracy classes are marked in different colors. The red lines correspond to the AA accuracy class limit, and the green ones correspond to the A+ accuracy class limit. The other limits of the accuracy classes are also marked.

The transition data from the GRASP2018 calculations, such as wavelengths, weighted oscillator strengths, line strengths, and transition rates of E1 transitions, are given in Table 6 along with the dT parameter, the $G_{S=0}$ parameter, and the estimated accuracy. The full table is available at the CDS.

The computed lifetimes for some levels are compared with experimental values and other theoretical calculations in Table 7. The GRASP2018 lifetimes of the $5p^6 6d \ ^2D$ are lower than the experimental values by 18% and 23% for $^2D_{3/2}$ and $^2D_{5/2}$, respectively. These lifetimes were recalculated using the experimental wavelengths for the radiative transition probabilities. This way, the errors stemming from uncertainties of the transition energies were eliminated, while the uncertainties coming from calculations of the line strength were estimated using the relative difference $(\tau_B - \tau_C)/\min(\tau_B, \tau_C)$ (Col. 1(adj.) in Table 7). Recalculated GRASP2018 lifetimes of the $5p^6 6d \ ^2D$ decreased a little, and the estimated uncertainty of calculations for these levels is about 29%. The HULLAC lifetimes for these levels are too low by 33% and 37% for $^2D_{3/2}$ and $^2D_{5/2}$, respectively. The lifetimes calculated by Savukov et al. (2003) are almost three times lower than the experimental ones. The lifetimes of the $5p^6 6p \ ^2P$

Fig. 28. Statistical evaluation of oscillator strength of E1 transitions from the present GRASP2018 and HULLAC computations.

Fig. 29. Statistical evaluation of wavelengths of E1 transitions from the present GRASP2018 and HULLAC computations.

levels in GRASP2018 have an uncertainty of about 3%, and they are in good agreement with other theoretical results.

Figures 28 and 29 show the statistical evaluation of oscillator strengths and wavelengths of E1 transitions from the GRASP2018 and HULLAC computations. GRASP2018 gives more transitions in the range of $\log(gf) < -3$, while HULLAC gives more transitions with $\log(gf) > -3$. The largest difference between the GRASP2018 and HULLAC results is in the range

Fig. 30. Expansion opacity (left) and the *Planck* mean opacity (right) calculated using the atomic data from the GRASP2018 and HULLAC calculations.

of $\log(gf) = (-3.4 \text{ to } -3.2)$. In the statistical distribution of the wavelengths, the difference between GRASP2018 and HULLAC results is not very large.

4. Opacities

The atomic data calculated from GRASP2018 and HULLAC are used here to calculate the bound-bound opacity of the material ejected in a binary NS merger. Here we assume that the ejected material consists of pure Ce and calculate the opacity of Ce IV by solving the ionization balance equations (see below). Although such a case does not represent a realistic condition, it helps us to understand the impact of the accuracy of atomic calculations on the opacity.

In NS mergers, the matter is expanding at high velocity with a high velocity gradient. As shown by Karp et al. (1977), the opacity can be enhanced by the expansion of the system. We use the expansion opacity formalism derived by Eastman & Pinto (1993):

$$\kappa_{\text{exp}}(\lambda) = \frac{1}{c\rho} \sum_l \frac{\lambda_l}{\Delta\lambda} (1 - e^{-\tau_l}), \quad (12)$$

where ρ is the density of the ejecta at time t , λ_l is the transition wavelength (l is the index of the line within the wavelength grid in the opacity calculations $\Delta\lambda$), and τ_l is the Sobolev optical depth at the transition wavelength. We use a linearly spaced wavelength grid of $\Delta\lambda = 10 \text{ \AA}$. Emission from the NS merger spans a wavelength range from ultraviolet to near-infrared (Metzger et al. 2010; Tanaka & Hotokezaka 2013; Kasen et al. 2013), and therefore we calculate the opacity in the wavelength range of $100\text{--}25\,000 \text{ \AA}$. Thus, our calculations have a wavelength resolution of $\Delta\lambda/\lambda \sim 0.1\text{--}0.0004$. We consider the density of the ejecta to be $\rho = 10^{-13} \text{ g cm}^{-3}$, which is the typical value at $t = 1$ day after the merger for a typical ejected mass of $0.01 M_\odot$. The Sobolev optical depth τ_l is calculated as

$$\tau_l = \frac{\pi e^2}{m_e c} n_{i,j} \lambda_l f_l t \frac{g_l}{g_0} e^{-\frac{E_l}{kT}}, \quad (13)$$

where e and m_e are the charge and the mass of an electron, k is the Boltzmann constant, $n_{i,j}$ is the number density of the j th ion

of the i th element, E_l , g_l , g_0 , and f_l are the energy, the statistical weight of the lower level and the ground state, and the oscillator strength of the transition. We note that the entire transition data set has been used for the calculation of opacity without any threshold imposed based on the transition strength. We assume local thermal equilibrium (LTE) for the calculation. The population in different energy levels is determined by the Boltzmann statistic, and the fraction of ionization for the given density is provided by solving the Saha ionization equation.

The expansion opacity is convolved with a blackbody function to calculate the *Planck* mean opacity as

$$\kappa_{\text{mean}} = \frac{\int_0^\infty \kappa_{\text{exp}}(\lambda) B_\lambda(T) d\lambda}{\int_0^\infty B_\lambda(T) d\lambda}. \quad (14)$$

The expansion opacity and the *Planck* mean opacity calculated from the GRASP2018 and HULLAC data are shown in Fig. 30. We note that Ce reaches the peak of the $3+$ ionization stage around the temperature range of $T \sim (10\,000\text{--}15\,000) \text{ K}$ for the given density ($\rho = 10^{-13} \text{ g cm}^{-3}$). Beyond $T = 20\,000 \text{ K}$, the number density of the Ce^{3+} is almost negligible. The expansion opacity at $T = 15\,000 \text{ K}$ is higher at shorter wavelengths. This is because the number of transitions is high at shorter wavelengths. The opacity spectra show different features for the cases of GRASP2018 and HULLAC data, which reflect the differences in the energy level distributions and transition wavelengths in the two calculations.

However, the overall properties of the opacities are similar: the *Planck* mean opacities derived from the atomic data calculated with GRASP2018 and HULLAC agree within 20 %. This is because mainly the strongest transitions contribute to the opacity, and these are not significantly different in the two calculations (Fig. 28). The *Planck* mean opacity increases with temperature, and reaches its maximum at around $T = 15\,000 \text{ K}$, beyond which it decreases. The maximum value of the *Planck* mean opacity is $\kappa_{\text{mean}} = 0.05 \text{ cm}^2 \text{ g}^{-1}$ and $0.06 \text{ cm}^2 \text{ g}^{-1}$ with the data of GRASP2018 and HULLAC, respectively.

The opacity presented in this work is much higher than found in previous studies on opacity of Ce IV (Tanaka et al. 2020; Carvajal Gallego et al. 2021). This is because the previous works used only a subset of the configurations used in this work. Therefore, the number of transitions in those previous studies was

Fig. 31. Effects of completeness of the atomic data on the *Planck* mean opacity. *Left panel:* Distribution of the energy levels from individual configurations as obtained from HULLAC. The number of energy levels inside 0.2 eV bins is represented as in the color scale. *Right panel:* *Planck* mean opacity as a function of temperature as calculated using the atomic data from HULLAC. The thick blue line is the opacity calculated using the full set of configurations, whereas the other lines correspond to the opacity calculated using only a subset of configurations. The opacity is unaffected by the removal of the energy levels corresponding to the configurations $5p^6 8s$, $5p^6 5g$, and so on down to $5p^5 4f 6s$ (the blue curves). However, further removal of the energy levels (e.g., those corresponding to the configurations $5p^6 5f$, $5p^6 6d$ and so on) results in a drop in the opacity (see red curves) from the default value calculated using the full atomic data (the thick blue curve).

small (16 and 37 in Tanaka et al. 2020 and Carvajal Gallego et al. 2021, respectively) in comparison to this work, where the number of transitions is 5056. This incompleteness of the atomic data affects the result of opacity calculation significantly.

To explore the effect of completeness of the atomic data on opacity in more detail, we performed a convergence test on the opacity calculation using only a subset of configurations (right panel in Fig. 31). We note that only the HULLAC data are used for this test. Our results show that removal of high-energy levels, that is, the energy levels of the configurations such as $5p^6 8s$, $5p^6 5g$, and so on down to $5p^5 4f 6s$ (see the left panel of Fig. 31), does not affect the opacity (see the blue curves in the right panel of Fig. 31). However, further removal of the energy levels results in a drop in the opacity (the red curves in the right panel of Fig. 31).

Transitions from relatively low energy levels (e.g., those from $5p^5 4f 5d$, $5p^5 4f^2$) to the high-energy levels corresponding to the configurations $5p^6 5f$, $5p^6 7s$, and $5p^6 6d$ are important, and hence removal of these energy levels affects the opacity. Transitions between the energy levels of the $5p^5 4f 5d$ and $5p^5 4f^2$ contribute significantly to the opacity. Transitions from the low-lying levels (e.g., from $5p^6 6p$) to the levels of the two configurations above them are also significant. Hence, without these energy levels, opacity is lower. Transitions between the low-lying energy levels have the most influence on the opacity. Therefore, removing all the energy levels of the configurations up to $5p^6 6p$ (the left panel of Fig. 31) causes almost an order of magnitude drop in opacity from the default value (calculated using the atomic data corresponding to the full set of configurations). Our convergence test highlights the importance of the complete atomic data for a realistic estimate of opacities.

5. Conclusions

We computed energy spectra for 225 levels and E1 transition data for the Ce^{3+} ion using the GRASP2018 and HULLAC codes. The HULLAC energy levels are higher than suggested by the NIST data: the rms deviations of the HULLAC results

from the NIST data are 5780 cm^{-1} . The energies computed with GRASP2018 are in good agreement with recommended values from the NIST ASD: the rms deviations are 1270 cm^{-1} . There is discrepancy in the order of the $5p^6 6d^2 D_{3/2,5/2}$ levels between the final GRASP2018 results and the NIST data. By analyzing the convergence and the quality of the wave functions for these levels, we find that our final results (with the $5p^6 6d^2 D_{3/2}$ level lower than $5p^6 6d^2 D_{5/2}$) are more accurate than results from other strategies.

Here, we developed the gauge dependency method, which can be used to evaluate the quality of the wave functions. This qualitative evaluation of the wave functions along with the agreement between both gauges was used to estimate the uncertainties of the computed line strengths. We also show that this method can be used to identify the transitions for which the ratio between the Babushkin and Coulomb gauges is a meaningful indicator of accuracy and those transitions for which the agreement between the two gauges is a random event not related to the real accuracy of the calculation.

As shown by the analysis of dependencies of line strengths on the gauge parameter G , the correlations included in the final computations (the VV3 strategy) are very important for all studied transitions. As the gauge dependencies are closer to linear when correlations included in the final computations (the VV3 strategy) are added, the wave functions of the final results should be more accurate than from other strategies. The analysis also showed that transition data in the Babushkin gauge are less affected by cancellation effects than data in other gauges.

Using the atomic data from GRASP2018 and HULLAC, the opacity in the ejecta from the NS merger is evaluated. The opacity spectra show different features, reflecting the difference in the energy level distributions and transition wavelengths in both data sets. However, the overall trend in the opacity is similar: the *Planck* mean opacities calculated with the GRASP2018 data agree with those with the HULLAC data within 20%. This means that the present atomic calculations provide a reasonable estimate of the overall opacity. The calculated opacity is significantly higher than those found in previous studies

(Tanaka et al. 2020; Carvajal Gallego et al. 2021). We believe this is due to the completeness of the atomic data corresponding to the higher number of configurations. However, we note that complete ab initio atomic calculations (up to the 31 eV energy limit for Ce IV) as presented in this paper are necessary for more elements and ions to fully understand the astrophysical opacity of lanthanide elements.

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Appendix A: Tables of atomic data for Ce IV.

The following Tables A.1 and A.2 list the results of the calculations discussed in the text.

Table A.1. Atomic state function composition (up to three *LS* components with a contribution > 0.02 of the total atomic state function) in *LS*-coupling and energy levels (in cm⁻¹) for Ce IV. Energy levels are given relative to the ground state. The labels for the levels marked in bold were not assigned by the largest contribution to the composition.

No.	State	<i>LS</i> -composition	<i>E_{RCI}</i>
1	$4f5s^25p^6\ ^2F_{5/2}^\circ$	0.95	0
2	$4f5s^25p^6\ ^2F_{7/2}^\circ$	0.95	2 053
3	$5s^25p^65d\ ^2D_{3/2}$	0.93	47 653
4	$5s^25p^65d\ ^2D_{5/2}$	0.93	50 163
5	$5s^25p^66s\ ^2S_{1/2}$	0.93	86 031
6	$5s^25p^66p\ ^2P_{1/2}^\circ$	0.93	121 809
7	$5s^25p^66p\ ^2P_{3/2}^\circ$	0.93	126 396
8	$4f^2(^3H)5s^25p^5\ ^4G_{5/2}^\circ$	$0.82 + 0.09\ 4f^2(^3F)5s^25p^5\ ^4G^\circ$	155 746
9	$4f^2(^3H)5s^25p^5\ ^4G_{7/2}^\circ$	$0.74 + 0.14\ 4f^2(^3F)5s^25p^5\ ^4G^\circ + 0.03\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	157 372
10	$4f^2(^3H)5s^25p^5\ ^4G_{9/2}^\circ$	$0.63 + 0.21\ 4f^2(^3F)5s^25p^5\ ^4G^\circ + 0.05\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	159 344
11	$4f^2(^3H)5s^25p^5\ ^4G_{11/2}^\circ$	$0.50 + 0.35\ 4f^2(^3F)5s^25p^5\ ^4G^\circ + 0.05\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	161 806
12	$4f^2(^3H)5s^25p^5\ ^4I_{15/2}^\circ$	0.95	164 825
13	$4f^2(^3H)5s^25p^5\ ^4I_{13/2}^\circ$	$0.79 + 0.13\ 4f^2(^3H)5s^25p^5\ ^2I^\circ + 0.03\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	165 132
14	$4f^2(^3F)5s^25p^5\ ^4D_{3/2}^\circ$	$0.59 + 0.21\ 4f^2(^3F)5s^25p^5\ ^4F^\circ + 0.11\ 4f^2(^3P)5s^25p^5\ ^4D^\circ$	165 793
15	$4f^2(^3H)5s^25p^5\ ^4I_{11/2}^\circ$	$0.59 + 0.28\ 4f^2(^3H)5s^25p^5\ ^2I^\circ + 0.04\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	165 827
16	$4f^2(^3F)5s^25p^5\ ^4D_{5/2}^\circ$	$0.47 + 0.31\ 4f^2(^3F)5s^25p^5\ ^4F^\circ + 0.12\ 4f^2(^3P)5s^25p^5\ ^4D^\circ$	165 896
17	$4f^2(^3F)5s^25p^5\ ^4D_{1/2}^\circ$	$0.81 + 0.11\ 4f^2(^3P)5s^25p^5\ ^4D^\circ$	166 283
18	$4f^2(^3F)5s^25p^5\ ^4D_{7/2}^\circ$	$0.32 + 0.28\ 4f^2(^3F)5s^25p^5\ ^4F^\circ + 0.13\ 4f^2(^3P)5s^25p^5\ ^4D^\circ$	166 392
19	$4f^2(^1G)5s^25p^5\ ^2F_{5/2}^\circ$	$0.49 + 0.14\ 4f^2(^3F)5s^25p^5\ ^2F^\circ + 0.08\ 4f^2(^3F)5s^25p^5\ ^4F^\circ$	167 854
20	$4f5s^25p^5(^3D)5d\ ^4G_{5/2}$	$0.74 + 0.10\ 4f5s^25p^5(^3G)5d\ ^4G + 0.07\ 4f5s^25p^5(^3F)5d\ ^4G$	168 330
21	$4f^2(^3F)5s^25p^5\ ^4F_{7/2}^\circ$	$0.24 + 0.23\ 4f^2(^1G)5s^25p^5\ ^2F^\circ + 0.18\ 4f^2(^1G)5s^25p^5\ ^2G^\circ$	168 582
22	$4f^2(^3H)5s^25p^5\ ^4I_{9/2}^\circ$	$0.35 + 0.17\ 4f^2(^3H)5s^25p^5\ ^4H^\circ + 0.11\ 4f^2(^3H)5s^25p^5\ ^2H^\circ$	168 601
23	$4f^2(^3F)5s^25p^5\ ^4F_{9/2}^\circ$	$0.62 + 0.11\ 4f^2(^3F)5s^25p^5\ ^4I^\circ + 0.07\ 4f^2(^3H)5s^25p^5\ ^2H^\circ$	169 659
24	$4f^2(^3F)5s^25p^5\ ^4F_{3/2}^\circ$	$0.48 + 0.18\ 4f^2(^3F)5s^25p^5\ ^2D^\circ + 0.15\ 4f^2(^3F)5s^25p^5\ ^4D^\circ$	171 575
25	$4f5s^25p^5(^3D)5d\ ^4G_{7/2}$	$0.66 + 0.17\ 4f5s^25p^5(^3G)5d\ ^4G + 0.05\ 4f5s^25p^5(^3F)5d\ ^4G$	171 681
26	$4f^2(^1G)5s^25p^5\ ^2H_{11/2}^\circ$	$0.83 + 0.03\ 4f^2(^3H)5s^25p^5\ ^2H^\circ + 0.03\ 4f^2(^3H)5s^25p^5\ ^4I^\circ$	171 824
27	$4f^2(^1G)5s^25p^5\ ^2G_{9/2}^\circ$	$0.41 + 0.16\ 4f^2(^3H)5s^25p^5\ ^2G^\circ + 0.15\ 4f^2(^1G)5s^25p^5\ ^2H^\circ$	172 009
28	$4f^2(^3H)5s^25p^5\ ^2I_{11/2}^\circ$	$0.43 + 0.30\ 4f^2(^3H)5s^25p^5\ ^4H^\circ + 0.08\ 4f^2(^3H)5s^25p^5\ ^2H^\circ$	172 590
29	$4f^2(^1G)5s^25p^5\ ^2G_{7/2}^\circ$	0.08 + $0.26\ 4f^2(^3H)5s^25p^5\ ^4H^\circ + 0.14\ 4f^2(^3H)5s^25p^5\ ^2G^\circ$	173 126
30	$4f5s^25p^5(^3D)5d\ ^4F_{3/2}$	$0.71 + 0.13\ 4f5s^25p^5(^3G)5d\ ^4F + 0.06\ 4f5s^25p^5(^3F)5d\ ^4F$	173 180
31	$4f^2(^3F)5s^25p^5\ ^4F_{5/2}^\circ$	$0.23 + 0.19\ 4f^2(^1G)5s^25p^5\ ^2F^\circ + 0.14\ 4f^2(^3F)5s^25p^5\ ^2D^\circ$	173 521
32	$4f5s^25p^5(^3D)5d\ ^4F_{5/2}$	$0.49 + 0.23\ 4f5s^25p^5(^3G)5d\ ^4F + 0.06\ 4f5s^25p^5(^3F)5d\ ^4F$	174 210
33	$4f^2(^3H)5s^25p^5\ ^4H_{13/2}^\circ$	$0.55 + 0.38\ 4f^2(^3H)5s^25p^5\ ^2I^\circ$	174 298
34	$4f5s^25p^5(^3D)5d\ ^4G_{9/2}$	$0.53 + 0.29\ 4f5s^25p^5(^3G)5d\ ^4G + 0.04\ 4f5s^25p^5(^3G)5d\ ^4F$	174 436
35	$4f5s^25p^5(^3D)5d\ ^4D_{3/2}$	$0.41 + 0.29\ 5s^25p^66d\ ^2D + 0.08\ 4f5s^25p^5(^3G)5d\ ^4D$	175 441
36	$5s^25p^66d\ ^2D_{3/2}$	$0.58 + 0.22\ 4f5s^25p^5(^3D)5d\ ^4D + 0.04\ 4f5s^25p^5(^3G)5d\ ^4D$	175 495
37	$4f5s^25p^5(^3D)5d\ ^4D_{5/2}$	$0.41 + 0.17\ 4f5s^25p^5(^3G)5d\ ^4D + 0.08\ 4f5s^25p^5(^3D)5d\ ^4F$	175 781
38	$4f5s^25p^5(^3D)5d\ ^4D_{1/2}$	$0.77 + 0.08\ 4f5s^25p^5(^3G)5d\ ^4D + 0.05\ 4f5s^25p^5(^3F)5d\ ^4D$	176 199
39	$5s^25p^66d\ ^2D_{5/2}$	$0.80 + 0.04\ 4f5s^25p^5(^3D)5d\ ^4D + 0.12\ 4f5s^25p^5(^3G)5d\ ^4D$	176 236
40	$4f^2(^3F)5s^25p^5\ ^4G_{9/2}^\circ$	$0.40 + 0.25\ 4f^2(^3F)5s^25p^5\ ^2G^\circ + 0.11\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	176 309
41	$4f^2(^3F)5s^25p^5\ ^2G_{7/2}^\circ$	$0.59 + 0.24\ 4f^2(^3F)5s^25p^5\ ^4G^\circ + 0.06\ 4f^2(^3H)5s^25p^5\ ^4G^\circ$	176 322
42	$4f5s^25p^5(^3G)5d\ ^4F_{7/2}$	$0.27 + 0.26\ 4f5s^25p^5(^3G)5d\ ^4D + 0.18\ 4f5s^25p^5(^3D)5d\ ^4F$	176 397
43	$4f5s^25p^5(^3D)5d\ ^2F_{5/2}$	$0.29 + 0.15\ 4f5s^25p^5(^3D)5d\ ^4F + 0.14\ 4f5s^25p^5(^1G)5d\ ^2F$	176 516
44	$4f^2(^3F)5s^25p^5\ ^4G_{11/2}^\circ$	$0.50 + 0.15\ 4f^2(^3H)5s^25p^5\ ^2H^\circ + 0.15\ 4f^2(^3H)5s^25p^5\ ^4G^\circ$	177 074
45	$4f5s^25p^5(^3D)5d\ ^4F_{7/2}$	$0.25 + 0.14\ 4f5s^25p^5(^1G)5d\ ^2F + 0.14\ 4f5s^25p^5(^3D)5d\ ^4D$	177 082
46	$4f^2(^3H)5s^25p^5\ ^4H_{7/2}^\circ$	$0.28 + 0.12\ 4f^2(^3F)5s^25p^5\ ^4F^\circ + 0.12\ 4f^2(^1G)5s^25p^5\ ^2F^\circ$	177 218
47	$4f^2(^1D)5s^25p^5\ ^2D_{5/2}^\circ$	$0.26 + 0.18\ 4f^2(^3P)5s^25p^5\ ^4P^\circ + 0.11\ 4f^2(^3F)5s^25p^5\ ^4F^\circ$	177 316
48	$4f5s^25p^5(^3G)5d\ ^4G_{11/2}$	$0.51 + 0.40\ 4f5s^25p^5(^3D)5d\ ^4G$	177 498
49	$4f^2(^3P)5s^25p^5\ ^2P_{5/2}^\circ$	$0.57 + 0.17\ 4f^2(^1D)5s^25p^5\ ^2D^\circ + 0.09\ 4f^2(^3F)5s^25p^5\ ^2D^\circ$	178 424
50	$4f5s^25p^5(^3G)5d\ ^4F_{9/2}$	$0.51 + 0.29\ 4f5s^25p^5(^3D)5d\ ^4F + 0.06\ 4f5s^25p^5(^3D)5d\ ^4G$	178 734
51	$4f^2(^1I)5s^25p^5\ ^2H_{9/2}^\circ$	$0.34 + 0.14\ 4f^2(^3H)5s^25p^5\ ^2G^\circ + 0.11\ 4f^2(^3H)5s^25p^5\ ^4H^\circ$	178 914
52	$4f^2(^1D)5s^25p^5\ ^2D_{3/2}^\circ$	0.23 + $0.27\ 4f^2(^3P)5s^25p^5\ ^4P^\circ + 0.18\ 4f^2(^1D)5s^25p^5\ ^2P^\circ$	179 047
53	$4f5s^25p^5(^3D)5d\ ^4P_{3/2}$	$0.51 + 0.19\ 4f5s^25p^5(^3D)5d\ ^4S + 0.05\ 4f5s^25p^5(^3D)5d\ ^2D$	179 097
54	$4f5s^25p^5(^3D)5d\ ^2F_{7/2}$	0.06 + $0.21\ 4f5s^25p^5(^3D)5d\ ^4F + 0.12\ 4f5s^25p^5(^1G)5d\ ^2F$	179 482
55	$4f5s^25p^5(^3D)5d\ ^4P_{5/2}$	$0.34 + 0.12\ 4f5s^25p^5(^3D)5d\ ^4D + 0.07\ 4f5s^25p^5(^3G)5d\ ^4D$	180 381
56	$4f5s^25p^5(^3G)5d\ ^4I_{15/2}$	0.97	180 860

Table A.1. Continued.

No.	State	LS-composition	E_{RCI}
57	$4f5s^25p^5(^3G)5d^2H_{11/2}$	$0.50 + 0.24 4f5s^25p^5(^1G)5d^2H + 0.06 4f5s^25p^5(^1F)5d^2H$	181 070
58	$4f5s^25p^5(^3D)5d^4P_{1/2}$	$0.81 + 0.04 4f5s^25p^5(^3F)5d^4D + 0.04 4f5s^25p^5(^3D)5d^2S$	181 098
59	$4f5s^25p^5(^3G)5d^4I_{13/2}$	$0.84 + 0.10 4f5s^25p^5(^1G)5d^2I$	181 357
60	$4f5s^25p^5(^3D)5d^2D_{3/2}$	$0.25 + 0.12 4f5s^25p^5(^3D)5d^2P + 0.11 4f5s^25p^5(^1F)5d^2D$	181 666
61	$4f^2(^3P)5s^25p^5^4P_{3/2}^o$	$0.51 + 0.19 4f^2(^1D)5s^25p^5^2D^o + 0.07 4f^2(^1D)5s^25p^5^2P^o$	181 732
62	$4f5s^25p^5(^1F)5d^2D_{5/2}$	0.16 + $0.29 4f5s^25p^5(^3D)5d^4P + 0.14 4f5s^25p^5(^1G)5d^2D$	182 504
63	$4f^2(^1I)5s^25p^5^2K_{5/2}^o$	0.93	182 519
64	$4f^2(^3P)5s^25p^5^4P_{1/2}^o$	$0.52 + 0.21 4f^2(^1D)5s^25p^5^2P^o + 0.09 4f^2(^3P)5s^25p^5^2P^o$	182 725
65	$4f5s^25p^5(^3G)5d^4I_{11/2}$	$0.65 + 0.15 4f5s^25p^5(^1G)5d^2I + 0.05 4f5s^25p^5(^3G)5d^2H$	182 803
66	$5s^25p^67s^2S_{1/2}$	0.90	182 938
67	$4f^2(^3H)5s^25p^5^4H_{9/2}$	0.25 + $0.27 4f^2(^1I)5s^25p^5^2H^o + 0.20 4f^2(^3H)5s^25p^5^4I^o$	183 182
68	$4f5s^25p^5(^3D)5d^4F_{9/2}$	$0.22 + 0.13 4f5s^25p^5(^3F)5d^4F + 0.09 4f5s^25p^5(^3F)5d^4G$	183 240
69	$4f5s^25p^5(^3G)5d^4D_{7/2}$	$0.38 + 0.19 4f5s^25p^5(^3D)5d^4D + 0.12 4f5s^25p^5(^3F)5d^4F$	183 632
70	$4f5s^25p^5(^3F)5d^4G_{9/2}$	0.02 + $0.14 4f5s^25p^5(^3D)5d^4F + 0.13 4f5s^25p^5(^1F)5d^2G$	183 895
71	$5s^25p^65f^2F_{5/2}^o$	$0.47 + 0.12 4f^2(^3F)5s^25p^5^4G^o + 0.11 4f^2(^3F)5s^25p^5^2F^o$	183 913
72	$4f5s^25p^5(^3G)5d^4H_{13/2}$	$0.84 + 0.12 4f5s^25p^5(^3F)5d^4H$	183 997
73	$5s^25p^65f^2F_{7/2}^o$	$0.54 + 0.20 4f^2(^1D)5s^25p^5^2F^o + 0.09 4f^2(^1G)5s^25p^5^2G^o$	184 167
74	$4f5s^25p^5(^3G)5d^4D_{3/2}$	0.18 + $0.23 4f5s^25p^5(^3D)5d^4S + 0.15 4f5s^25p^5(^3D)5d^4D$	184 218
75	$4f5s^25p^5(^3G)5d^4D_{5/2}$	$0.28 + 0.20 4f5s^25p^5(^3D)5d^2D + 0.19 4f5s^25p^5(^3F)5d^4F$	184 344
76	$4f^2(^3F)5s^25p^5^2F_{5/2}^o$	0.11 + $0.45 5s^25p^65f^2F^o + 0.15 4f^2(^3F)5s^25p^5^4G^o$	184 414
77	$4f5s^25p^5(^3G)5d^4H_{11/2}$	$0.66 + 0.11 4f5s^25p^5(^3F)5d^4H + 0.08 4f5s^25p^5(^3G)5d^2H$	184 439
78	$4f^2(^1D)5s^25p^5^2F_{7/2}^o$	0.31 + $0.37 5s^25p^65f^2F^o + 0.14 4f^2(^1G)5s^25p^5^2G^o$	184 491
79	$4f5s^25p^5(^3D)5d^2P_{1/2}$	$0.59 + 0.12 4f5s^25p^5(^3G)5d^4D + 0.09 4f5s^25p^5(^3F)5d^2P$	184 882
80	$4f5s^25p^5(^3D)5d^2G_{7/2}$	$0.25 + 0.24 4f5s^25p^5(^1G)5d^2G + 0.10 4f5s^25p^5(^3G)5d^4H$	184 924
81	$4f5s^25p^5(^3G)5d^4H_{9/2}$	$0.30 + 0.16 4f5s^25p^5(^3G)5d^2H + 0.10 4f5s^25p^5(^3F)5d^4H$	185 497
82	$4f^2(^1D)5s^25p^5^2P_{1/2}^o$	$0.50 + 0.28 4f^2(^3P)5s^25p^5^4P^o + 0.05 4f^2(^3P)5s^25p^5^2P^o$	185 955
83	$4f5s^25p^5(^1G)5d^2D_{3/2}$	$0.16 + 0.15 4f5s^25p^5(^3F)5d^4F + 0.11 4f5s^25p^5(^3D)5d^4S$	186 260
84	$4f5s^25p^5(^3D)5d^4D_{7/2}$	$0.23 + 0.16 4f5s^25p^5(^3F)5d^4G + 0.15 4f5s^25p^5(^1F)5d^2G$	186 491
85	$4f5s^25p^5(^3G)5d^4I_{9/2}$	$0.65 + 0.11 4f5s^25p^5(^1F)5d^2H + 0.09 4f5s^25p^5(^3F)5d^4H$	186 595
86	$4f5s^25p^5(^3D)5d^2D_{5/2}$	$0.23 + 0.15 4f5s^25p^5(^1F)5d^2F + 0.11 4f5s^25p^5(^3D)5d^2F$	187 070
87	$4f^2(^3F)5s^25p^5^2F_{7/2}^o$	$0.34 + 0.22 4f^2(^3P)5s^25p^5^4D^o + 0.13 4f^2(^1G)5s^25p^5^2G^o$	187 254
88	$4f5s^25p^5(^3G)5d^2F_{7/2}$	$0.27 + 0.13 4f5s^25p^5(^1F)5d^2G + 0.12 4f5s^25p^5(^1G)5d^2F$	187 267
89	$4f5s^25p^5(^3D)5d^4S_{3/2}$	$0.25 + 0.11 4f5s^25p^5(^3D)5d^2P + 0.10 4f5s^25p^5(^3F)5d^4F$	187 374
90	$4f5s^25p^5(^3G)5d^4F_{5/2}$	0.02 + $0.21 4f5s^25p^5(^3D)5d^4D + 0.13 4f5s^25p^5(^3D)5d^4P$	187 760
91	$4f5s^25p^5(^3G)5d^4G_{9/2}$	0.15 + $0.28 4f5s^25p^5(^1G)5d^2G + 0.12 4f5s^25p^5(^3F)5d^4G$	187 795
92	$4f^2(^1D)5s^25p^5^2H_{11/2}^o$	$0.39 + 0.14 4f^2(^3H)5s^25p^5^2H^o + 0.09 4f^2(^3H)5s^25p^5^2I^o$	188 174
93	$4f5s^25p^5(^3G)5d^4D_{1/2}$	$0.33 + 0.15 4f5s^25p^5(^3D)5d^4D + 0.12 4f5s^25p^5(^3F)5d^4D$	189 055
94	$4f5s^25p^5(^1F)5d^2D_{3/2}$	0.04 + $0.22 4f5s^25p^5(^3D)5d^2D + 0.17 4f5s^25p^5(^3G)5d^4D$	189 600
95	$4f5s^25p^5(^3F)5d^4G_{11/2}$	$0.35 + 0.27 4f5s^25p^5(^3G)5d^4G + 0.18 4f5s^25p^5(^3D)5d^4G$	189 677
96	$4f5s^25p^5(^1G)5d^2G_{7/2}$	$0.16 + 0.13 4f5s^25p^5(^3F)5d^4G + 0.12 4f5s^25p^5(^3D)5d^2F$	189 799
97	$4f^2(^3H)5s^25p^5^4H_{11/2}^o$	$0.46 + 0.17 4f^2(^3H)5s^25p^5^4I^o + 0.13 4f^2(^3H)5s^25p^5^4G^o$	189 971
98	$4f^2(^3H)5s^25p^5^2H_{9/2}^o$	$0.35 + 0.24 4f^2(^1G)5s^25p^5^2H^o + 0.16 4f^2(^1G)5s^25p^5^2G^o$	190 243
99	$4f5s^25p^5(^1D)5d^2G_{7/2}$	$0.15 + 0.13 4f5s^25p^5(^3F)5d^2F + 0.13 4f5s^25p^5(^3G)5d^2G$	191 127
100	$4f5s^25p^5(^3G)5d^2G_{9/2}$	$0.24 + 0.20 4f5s^25p^5(^3F)5d^4G + 0.13 4f5s^25p^5(^1G)5d^2H$	191 184
101	$4f^2(^1I)5s^25p^5^2K_{13/2}^o$	$0.56 + 0.24 4f^2(^1I)5s^25p^5^2I^o + 0.05 4f^2(^3H)5s^25p^5^2I^o$	191 185
102	$4f5s^25p^5(^1G)5d^2H_{9/2}$	0.17 + $0.18 4f5s^25p^5(^3G)5d^2G + 0.11 4f5s^25p^5(^1F)5d^2G$	191 435
103	$4f5s^25p^5(^3F)5d^4G_{5/2}$	$0.25 + 0.11 4f5s^25p^5(^1G)5d^2D + 0.09 4f5s^25p^5(^1D)5d^2F$	191 897
104	$4f^2(^3P)5s^25p^5^2D_{3/2}^o$	$0.31 + 0.15 4f^2(^3F)5s^25p^5^2D^o + 0.12 4f^2(^1D)5s^25p^5^2P^o$	192 193
105	$4f5s^25p^5(^3G)5d^4G_{7/2}$	$0.19 + 0.17 4f5s^25p^5(^3D)5d^2G + 0.15 4f5s^25p^5(^3G)5d^4F$	192 478
106	$4f^2(^3H)5s^25p^5^2G_{9/2}^o$	$0.26 + 0.19 4f^2(^3H)5s^25p^5^4H^o + 0.17 4f^2(^1G)5s^25p^5^2H^o$	192 639
107	$4f^2(^3H)5s^25p^5^2I_{13/2}^o$	$0.38 + 0.32 4f^2(^3H)5s^25p^5^4H^o + 0.12 4f^2(^3H)5s^25p^5^4I^o$	192 660
108	$4f5s^25p^5(^3D)5d^4G_{11/2}$	0.12 + $0.32 4f5s^25p^5(^3F)5d^4G + 0.20 4f5s^25p^5(^1G)5d^2H$	192 717
109	$4f^2(^3P)5s^25p^5^4D_{5/2}^o$	0.25 + $0.26 4f^2(^3F)5s^25p^5^2D^o + 0.19 4f^2(^3P)5s^25p^5^2D^o$	192 723
110	$4f5s^25p^5(^1G)5d^2I_{13/2}$	$0.51 + 0.35 4f5s^25p^5(^3G)5d^2I + 0.08 4f5s^25p^5(^3F)5d^4H$	193 271
111	$4f5s^25p^5(^1G)5d^2I_{11/2}$	$0.41 + 0.13 4f5s^25p^5(^3F)5d^4H + 0.08 4f5s^25p^5(^1F)5d^2H$	193 875
112	$4f^2(^3F)5s^25p^5^4G_{7/2}^o$	$0.30 + 0.24 4f^2(^3F)5s^25p^5^2G^o + 0.11 4f^2(^1G)5s^25p^5^2F^o$	193 881
113	$4f5s^25p^5(^3F)5d^4F_{9/2}$	$0.24 + 0.21 4f5s^25p^5(^3G)5d^4F + 0.16 4f5s^25p^5(^3D)5d^2G$	194 012
114	$4f5s^25p^5(^1D)5d^2F_{5/2}$	$0.17 + 0.15 4f5s^25p^5(^3G)5d^4G + 0.14 4f5s^25p^5(^3G)5d^4F$	194 299
115	$4f^2(^3P)5s^25p^5^2P_{3/2}^o$	0.16 + $0.21 4f^2(^3P)5s^25p^5^2D^o + 0.19 4f^2(^1D)5s^25p^5^2D^o$	195 482
116	$4f^2(^3F)5s^25p^5^4G_{5/2}^o$	$0.43 + 0.34 4f^2(^3F)5s^25p^5^2F^o + 0.03 4f^2(^3H)5s^25p^5^4G^o$	195 711
117	$4f5s^25p^5(^3F)5d^4G_{7/2}$	0.05 + $0.14 4f5s^25p^5(^3F)5d^2F + 0.12 4f5s^25p^5(^3F)5d^4H$	195 959
118	$4f^2(^3P)5s^25p^5^2P_{1/2}^o$	0.30 + $0.44 5s^25p^67p^2P^o + 0.08 4f^2(^3P)5s^25p^5^4D^o$	196 348
119	$4f5s^25p^5(^3D)5d^2S_{1/2}$	$0.68 + 0.10 4f5s^25p^5(^3F)5d^2P + 0.06 4f5s^25p^5(^1F)5d^2P$	196 583
120	$4f^2(^3F)5s^25p^5^2G_{9/2}^o$	$0.47 + 0.24 4f^2(^3F)5s^25p^5^4G^o + 0.10 4f^2(^3F)5s^25p^5^4F^o$	196 816
121	$4f5s^25p^5(^1D)5d^2D_{5/2}$	$0.24 + 0.09 4f5s^25p^5(^3F)5d^4F + 0.09 4f5s^25p^5(^1G)5d^2F$	196 982
122	$4f^2(^3H)5s^25p^5^2H_{11/2}^o$	$0.46 + 0.19 4f^2(^1I)5s^25p^5^2H^o + 0.14 4f^2(^1I)5s^25p^5^2I^o$	197 430

Table A.1. Continued.

No.	State	LS-composition	E_{RC1}
123	$4f5s^25p^5(^3G)5d^2I_{13/2}$	$0.46 + 0.34 4f5s^25p^5(^3F)5d^4H + 0.09 4f5s^25p^5(^1G)5d^2I$	197 750
124	$4f^2(^3H)5s^25p^5(^2G)_{7/2}^o$	$0.34 + 0.13 4f^2(^3H)5s^25p^5(^4H^o) + 0.09 4f^2(^3F)5s^25p^5(^4G^o)$	198 173
125	$4f5s^25p^5(^3D)5d^2P_{3/2}$	$0.34 + 0.14 4f5s^25p^5(^1G)5d^2D + 0.14 4f5s^25p^5(^3D)5d^2D$	198 260
126	$4f5s^25p^5(^1D)5d^2D_{3/2}$	$0.29 + 0.13 4f5s^25p^5(^3G)5d^4F + 0.12 4f5s^25p^5(^1F)5d^2D$	198 547
127	$4f5s^25p^5(^3F)5d^4F_{7/2}$	$0.12 + 0.15 4f5s^25p^5(^3D)5d^2G + 0.12 4f5s^25p^5(^1D)5d^2F$	198 582
128	$5s^25p^67p^2P_{3/2}^o$	$0.75 + 0.08 4f^2(^3P)5s^25p^5(^2P^o) + 0.03 4f^2(^3P)5s^25p^5(^4S^o)$	198 811
129	$5s^25p^67p^2P_{1/2}^o$	$0.48 + 0.20 4f^2(^3P)5s^25p^5(^2P^o) + 0.09 4f^2(^3P)5s^25p^5(^4D^o)$	198 816
130	$4f5s^25p^5(^1G)5d^2F_{5/2}$	$0.24 + 0.14 4f5s^25p^5(^3F)5d^4D + 0.09 4f5s^25p^5(^3G)5d^4G$	200 055
131	$4f^2(^1G)5s^25p^5(^2H)_{9/2}^o$	$0.20 + 0.25 4f^2(^3H)5s^25p^5(^2G^o) + 0.18 4f^2(^1G)5s^25p^5(^2G^o)$	201 234
132	$4f5s^25p^5(^3G)5d^4G_{5/2}$	$0.34 + 0.09 4f5s^25p^5(^3F)5d^4F + 0.08 4f5s^25p^5(^1F)5d^2F$	201 337
133	$4f^2(^3P)5s^25p^5(^4D)_{7/2}^o$	$0.18 + 0.21 4f^2(^3F)5s^25p^5(^4D^o) + 0.17 4f^2(^3H)5s^25p^5(^2G^o)$	201 403
134	$4f^2(^3F)5s^25p^5(^2S)_{3/2}^o$	$0.27 + 0.15 4f^2(^1D)5s^25p^5(^2F^o) + 0.15 4f^2(^3F)5s^25p^5(^4D^o)$	201 476
135	$4f5s^25p^5(^1D)5d^2P_{3/2}$	$0.46 + 0.22 4f5s^25p^5(^3F)5d^4P + 0.10 4f5s^25p^5(^3F)5d^4D$	201 988
136	$4f^2(^3F)5s^25p^5(^2D)_{3/2}^o$	$0.37 + 0.15 4f^2(^3P)5s^25p^5(^2D^o) + 0.10 5s^25p^67p^2P^o$	201 990
137	$4f5s^25p^5(^1D)5d^2G_{9/2}$	$0.19 + 0.18 4f5s^25p^5(^3G)5d^2H + 0.10 4f5s^25p^5(^3F)5d^4H$	202 208
138	$4f5s^25p^5(^3G)5d^2I_{11/2}$	$0.48 + 0.19 4f5s^25p^5(^3F)5d^2H + 0.14 4f5s^25p^5(^1F)5d^2H$	202 354
139	$4f5s^25p^5(^3G)5d^4H_{7/2}$	$0.35 + 0.16 4f5s^25p^5(^3F)5d^4G + 0.10 4f5s^25p^5(^1D)5d^2F$	202 535
140	$4f5s^25p^5(^1D)5d^2P_{1/2}$	$0.38 + 0.21 4f5s^25p^5(^3F)5d^4D + 0.10 4f5s^25p^5(^1F)5d^2P$	202 592
141	$4f5s^25p^5(^3G)5d^2H_{9/2}$	$0.19 + 0.18 4f5s^25p^5(^3D)5d^2G + 0.14 4f5s^25p^5(^1G)5d^2H$	203 213
142	$4f^2(^1G)5s^25p^5(^2F)_{7/2}^o$	$0.21 + 0.28 4f^2(^3F)5s^25p^5(^2F^o) + 0.16 4f^2(^3F)5s^25p^5(^4D^o)$	204 368
143	$4f5s^25p^5(^1D)5d^2S_{1/2}$	$0.53 + 0.33 4f5s^25p^5(^3F)5d^4P + 0.04 4f5s^25p^5(^3F)5d^2P$	204 458
144	$4f5s^25p^5(^3F)5d^4H_{7/2}$	$0.15 + 0.13 4f5s^25p^5(^3F)5d^4D + 0.08 4f5s^25p^5(^3G)5d^4G$	204 521
145	$4f^2(^1D)5s^25p^5(^2P)_{3/2}^o$	$0.09 + 0.19 4f^2(^3F)5s^25p^5(^2D^o) + 0.16 4f^2(^1S)5s^25p^5(^2P^o)$	204 760
146	$4f5s^25p^5(^1F)5d^2G_{7/2}$	$0.24 + 0.20 4f5s^25p^5(^3G)5d^4G + 0.13 4f5s^25p^5(^3G)5d^4H$	206 362
147	$4f5s^25p^5(^3G)5d^4F_{3/2}$	$0.20 + 0.18 4f5s^25p^5(^1F)5d^2D + 0.11 4f5s^25p^5(^3F)5d^4D$	206 891
148	$4f5s^25p^5(^3D)5d^2G_{9/2}$	$0.03 + 0.18 4f5s^25p^5(^3G)5d^4H + 0.17 4f5s^25p^5(^1F)5d^2H$	206 972
149	$4f5s^25p^5(^3F)5d^4D_{5/2}$	$0.15 + 0.11 4f5s^25p^5(^3F)5d^4P + 0.11 4f5s^25p^5(^3F)5d^2D$	207 106
150	$4f^2(^1D)5s^25p^5(^2F)_{5/2}^o$	$0.56 + 0.13 4f^2(^1D)5s^25p^5(^2D^o) + 0.09 4f^2(^3F)5s^25p^5(^2D^o)$	208 053
151	$4f5s^25p^5(^3G)5d^2F_{5/2}$	$0.24 + 0.19 4f5s^25p^5(^3F)5d^2F + 0.12 4f5s^25p^5(^1F)5d^2D$	208 481
152	$4f5s^25p^5(^3F)5d^4H_{9/2}$	$0.33 + 0.13 4f5s^25p^5(^3F)5d^4G + 0.10 4f5s^25p^5(^3G)5d^4I$	208 883
153	$4f5s^25p^5(^3D)6s^4D_{3/2}$	$0.78 + 0.13 4f5s^25p^5(^3D)6s^2D$	208 903
154	$4f5s^25p^5(^3D)6s^4D_{1/2}$	0.93	208 952
155	$4f5s^25p^5(^3G)5d^2G_{7/2}$	$0.13 + 0.14 4f5s^25p^5(^1D)5d^2G + 0.13 4f5s^25p^5(^3F)5d^4H$	209 560
156	$4f5s^25p^5(^3F)5d^4D_{7/2}$	$0.17 + 0.15 4f5s^25p^5(^1F)5d^2F + 0.13 4f5s^25p^5(^3F)5d^4H$	210 556
157	$4f5s^25p^5(^1F)5d^2H_{9/2}$	$0.19 + 0.17 4f5s^25p^5(^3G)5d^4H + 0.09 4f5s^25p^5(^3F)5d^4G$	210 803
158	$4f5s^25p^5(^1G)5d^2H_{11/2}$	$0.21 + 0.17 4f5s^25p^5(^3F)5d^4H + 0.13 4f5s^25p^5(^3G)5d^4I$	211 346
159	$4f5s^25p^5(^3D)6s^4D_{5/2}$	$0.54 + 0.08 4f5s^25p^5(^3F)5d^4P + 0.06 4f5s^25p^5(^3D)6s^2D$	211 443
160	$4f5s^25p^5(^3G)5d^4F_{5/2}$	$0.12 + 0.16 4f5s^25p^5(^1G)5d^2F + 0.11 4f5s^25p^5(^1D)5d^2F$	211 488
161	$4f^2(^3P)5s^25p^5(^4D)_{1/2}^o$	$0.49 + 0.24 4f^2(^3P)5s^25p^5(^2S^o) + 0.07 4f^2(^3P)5s^25p^5(^2P^o)$	211 741
162	$4f^2(^3P)5s^25p^5(^4D)_{3/2}^o$	$0.43 + 0.18 4f^2(^3P)5s^25p^5(^2D^o) + 0.15 4f^2(^3P)5s^25p^5(^4S^o)$	212 244
163	$4f5s^25p^5(^3F)5d^4F_{3/2}$	$0.26 + 0.22 4f5s^25p^5(^1D)5d^2D + 0.10 4f5s^25p^5(^3D)6s^2D$	212 428
164	$4f5s^25p^5(^1D)5d^2F_{7/2}$	$0.16 + 0.15 4f5s^25p^5(^3F)5d^4D + 0.08 4f5s^25p^5(^1F)5d^2F$	212 553
165	$4f5s^25p^5(^1G)5d^2G_{9/2}$	$0.31 + 0.10 4f5s^25p^5(^3G)5d^4G + 0.09 4f5s^25p^5(^3F)5d^2G$	212 579
166	$4f^2(^1D)5s^25p^5(^2F)_{13/2}^o$	$0.66 + 0.25 4f^2(^1D)5s^25p^5(^2K^o)$	212 653
167	$4f5s^25p^5(^1F)5d^2F_{5/2}$	$0.10 + 0.17 4f5s^25p^5(^3D)6s^4D + 0.11 4f5s^25p^5(^1F)5d^2D$	212 700
168	$4f5s^25p^5(^3F)5d^4H_{11/2}$	$0.33 + 0.16 4f5s^25p^5(^3G)5d^4H + 0.11 4f5s^25p^5(^1G)5d^2H$	212 892
169	$4f5s^25p^5(^3D)6s^2D_{3/2}$	$0.53 + 0.08 4f5s^25p^5(^3D)6s^4D + 0.08 4f5s^25p^5(^1D)5d^2D$	213 087
170	$4f5s^25p^5(^3F)5d^2P_{3/2}$	$0.32 + 0.22 4f5s^25p^5(^1F)5d^2D + 0.13 4f5s^25p^5(^3D)6s^2D$	213 477
171	$4f^2(^3P)5s^25p^5(^2D)_{5/2}^o$	$0.52 + 0.30 4f^2(^3P)5s^25p^5(^4D^o) + 0.05 4f^2(^3F)5s^25p^5(^4D^o)$	213 647
172	$4f^2(^3P)5s^25p^5(^2S)_{1/2}^o$	$0.50 + 0.19 4f^2(^3P)5s^25p^5(^2P^o) + 0.13 4f^2(^3P)5s^25p^5(^4D^o)$	214 624
173	$4f5s^25p^5(^1F)5d^2P_{3/2}$	$0.46 + 0.08 4f5s^25p^5(^1D)5d^2D + 0.07 4f5s^25p^5(^3F)5d^2P$	214 788
174	$4f^2(^1D)5s^25p^5(^2F)_{11/2}^o$	$0.67 + 0.23 4f^2(^1D)5s^25p^5(^2H^o)$	214 829
175	$4f5s^25p^5(^1F)5d^2H_{11/2}$	$0.46 + 0.11 4f5s^25p^5(^3D)5d^4G + 0.09 4f5s^25p^5(^3F)5d^2H$	215 110
176	$4f5s^25p^5(^1F)5d^2G_{9/2}$	$0.15 + 0.17 4f5s^25p^5(^1D)5d^2G + 0.11 4f5s^25p^5(^1F)5d^2H$	215 267
177	$4f5s^25p^5(^3F)5d^4H_{13/2}$	$0.40 + 0.26 4f5s^25p^5(^1G)5d^2I + 0.14 4f5s^25p^5(^3G)5d^2I$	216 002
178	$4f5s^25p^5(^3F)5d^4P_{5/2}$	$0.42 + 0.10 4f5s^25p^5(^3F)5d^4D + 0.06 4f5s^25p^5(^3F)5d^2D$	216 063
179	$4f5s^25p^5(^3G)6s^4G_{11/2}$	$0.85 + 0.02 4f5s^25p^5(^3F)5d^4G$	216 312
180	$4f5s^25p^5(^3G)6s^4G_{9/2}$	$0.50 + 0.23 4f5s^25p^5(^1G)6s^2G + 0.04 4f5s^25p^5(^3G)6s^2G$	216 616
181	$4f5s^25p^5(^1F)5d^2P_{1/2}$	$0.46 + 0.17 4f5s^25p^5(^3G)5d^4D + 0.14 4f5s^25p^5(^3F)5d^2P$	216 680
182	$4f^2(^1S)5s^25p^5(^2P)_{3/2}^o$	$0.40 + 0.37 4f^2(^1D)5s^25p^5(^2P^o) + 0.06 4f^2(^1D)5s^25p^5(^2D^o)$	216 718
183	$4f5s^25p^5(^1F)5d^2F_{7/2}$	$0.04 + 0.16 4f5s^25p^5(^3G)6s^4G + 0.15 4f5s^25p^5(^1D)5d^2F$	217 118
184	$4f5s^25p^5(^3D)6s^4D_{7/2}$	$0.49 + 0.08 4f5s^25p^5(^3F)6s^4F + 0.06 4f5s^25p^5(^1D)5d^2F$	217 340
185	$4f5s^25p^5(^1G)5d^2D_{5/2}$	$0.05 + 0.17 4f5s^25p^5(^1D)5d^2D + 0.14 4f5s^25p^5(^3F)5d^2F$	217 545
186	$4f5s^25p^5(^3F)5d^4P_{3/2}$	$0.33 + 0.14 4f5s^25p^5(^3F)5d^4D + 0.12 4f5s^25p^5(^3G)5d^4D$	218 093
187	$4f5s^25p^5(^3G)6s^4G_{7/2}$	$0.36 + 0.21 4f5s^25p^5(^1G)6s^2G + 0.10 4f5s^25p^5(^3G)6s^2G$	218 144
188	$4f^2(^3P)5s^25p^5(^4S)_{3/2}^o$	$0.47 + 0.30 4f^2(^3P)5s^25p^5(^2P^o) + 0.04 4f^2(^1S)5s^25p^5(^2P^o)$	218 147
189	$4f5s^25p^5(^3G)6s^2G_{9/2}$	$0.74 + 0.14 4f5s^25p^5(^3G)6s^4G + 0.05 4f5s^25p^5(^1G)6s^2G$	218 354

Table A.1. Continued.

No.	State	LS-composition	E_{RCI}
190	$4f 5s^2 5p^5(^3D) 6s^2 D_{5/2}$	$0.49 + 0.09 4f 5s^2 5p^5(^1F) 5d^2 D + 0.08 4f 5s^2 5p^5(^3F) 6s^2 F$	218 419
191	$4f 5s^2 5p^5(^1G) 5d^2 F_{7/2}$	$0.18 + 0.11 4f 5s^2 5p^5(^3F) 5d^2 G + 0.11 4f 5s^2 5p^5(^3G) 5d^2 G$	218 831
192	$4f 5s^2 5p^5(^3F) 5d^4 D_{1/2}$	$0.40 + 0.22 4f 5s^2 5p^5(^1D) 5d^2 P + 0.14 4f 5s^2 5p^5(^3G) 5d^4 D$	219 095
193	$4f 5s^2 5p^5(^3F) 5d^2 D_{5/2}$	$0.22 + 0.16 4f 5s^2 5p^5(^1D) 5d^2 D + 0.10 4f 5s^2 5p^5(^3F) 5d^4 D$	219 585
194	$4f 5s^2 5p^5(^3G) 6s^4 G_{5/2}$	$0.49 + 0.25 4f 5s^2 5p^5(^1F) 6s^2 F + 0.12 4f 5s^2 5p^5(^3F) 6s^4 F$	221 098
195	$5s^2 5p^6 7d^2 D_{3/2}$	0.84	221 463
196	$4f 5s^2 5p^5(^3F) 5d^4 D_{3/2}$	$0.11 + 0.28 4f 5s^2 5p^5(^1D) 5d^2 P + 0.22 4f 5s^2 5p^5(^3F) 5d^4 P$	221 885
197	$5s^2 5p^6 7d^2 D_{5/2}$	0.86	221 952
198	$4f 5s^2 5p^5(^3G) 6s^2 G_{7/2}$	$0.37 + 0.30 4f 5s^2 5p^5(^1F) 6s^2 F + 0.12 4f 5s^2 5p^5(^3F) 6s^4 F$	222 645
199	$4f 5s^2 5p^5(^3F) 5d^4 P_{1/2}$	$0.37 + 0.16 4f 5s^2 5p^5(^1D) 5d^2 S + 0.15 5s^2 5p^6 8s^2 S$	223 332
200	$4f 5s^2 5p^5(^3F) 5d^2 H_{11/2}$	$0.45 + 0.27 4f 5s^2 5p^5(^3G) 5d^2 I + 0.07 4f 5s^2 5p^5(^1G) 5d^2 H$	223 614
201	$4f 5s^2 5p^5(^3F) 5d^2 H_{9/2}$	$0.48 + 0.18 4f 5s^2 5p^5(^1D) 5d^2 G + 0.06 5s^2 5p^6 5g^2 G$	224 226
202	$4f 5s^2 5p^5(^3F) 5d^2 D_{3/2}$	$0.28 + 0.19 4f 5s^2 5p^5(^3F) 5d^2 P + 0.17 4f 5s^2 5p^5(^1G) 5d^2 D$	224 461
203	$5s^2 5p^6 8s^2 S_{1/2}$	$0.73 + 0.06 4f 5s^2 5p^5(^3F) 5d^4 P + 0.04 4f 5s^2 5p^5(^1F) 5d^2 P$	225 137
204	$5s^2 5p^6 5g^2 G_{7/2}$	0.93	225 466
205	$5s^2 5p^6 5g^2 G_{9/2}$	$0.69 + 0.13 4f 5s^2 5p^5(^3F) 6s^4 F + 0.07 4f 5s^2 5p^5(^1G) 6s^2 G$	225 794
206	$4f 5s^2 5p^5(^3F) 6s^4 F_{9/2}$	$0.40 + 0.24 4f 5s^2 5p^5(^1G) 6s^2 G + 0.18 5s^2 5p^6 5g^2 G$	226 020
207	$4f 5s^2 5p^5(^1G) 6s^2 G_{7/2}$	$0.39 + 0.33 4f 5s^2 5p^5(^3F) 6s^2 F + 0.13 4f 5s^2 5p^5(^3F) 6s^4 F$	226 577
208	$4f 5s^2 5p^5(^3F) 5d^2 P_{1/2}$	$0.45 + 0.12 4f 5s^2 5p^5(^3D) 5d^2 P + 0.12 4f 5s^2 5p^5(^1F) 5d^2 P$	226 730
209	$4f 5s^2 5p^5(^3F) 6s^4 F_{3/2}$	$0.47 + 0.43 4f 5s^2 5p^5(^1D) 6s^2 D$	227 511
210	$4f 5s^2 5p^5(^1D) 6s^2 D_{5/2}$	$0.49 + 0.21 4f 5s^2 5p^5(^3F) 6s^4 F + 0.20 4f 5s^2 5p^5(^3F) 6s^2 F$	228 543
211	$4f^2(^1S) 5s^2 5p^5(^2P^o)_{1/2}$	$0.79 + 0.05 4f^2(^1D) 5s^2 5p^5(^2P^o) + 0.03 5s^2 5p^5(^2P) 5d^2(^1S)^2 P^o$	231 894
212	$4f 5s^2 5p^5(^1F) 6s^2 F_{5/2}$	$0.42 + 0.40 4f 5s^2 5p^5(^3G) 6s^4 G + 0.07 4f 5s^2 5p^5(^3F) 6s^4 F$	240 581
213	$4f 5s^2 5p^5(^1F) 6s^2 F_{7/2}$	0.29 + $0.32 4f 5s^2 5p^5(^3G) 6s^2 G + 0.19 4f 5s^2 5p^5(^3G) 6s^4 G$	241 889
214	$4f 5s^2 5p^5(^3F) 6s^4 F_{5/2}$	$0.29 + 0.21 4f 5s^2 5p^5(^3F) 6s^2 F + 0.19 4f 5s^2 5p^5(^3D) 6s^2 D$	243 774
215	$4f 5s^2 5p^5(^3F) 6s^4 F_{7/2}$	$0.42 + 0.19 4f 5s^2 5p^5(^1F) 6s^2 F + 0.14 4f 5s^2 5p^5(^3D) 6s^4 D$	244 287
216	$4f 5s^2 5p^5(^1G) 6s^2 G_{9/2}$	0.31 + $0.37 4f 5s^2 5p^5(^3F) 6s^4 F + 0.17 4f 5s^2 5p^5(^3G) 6s^4 G$	245 567
217	$4f 5s^2 5p^5(^3F) 6s^2 F_{7/2}$	$0.49 + 0.15 4f 5s^2 5p^5(^1G) 6s^2 G + 0.09 4f 5s^2 5p^5(^1F) 6s^2 F$	246 746
218	$4f 5s^2 5p^5(^1D) 6s^2 D_{3/2}$	$0.41 + 0.34 4f 5s^2 5p^5(^3F) 6s^4 F + 0.06 4f 5s^2 5p^5(^3G) 5d^2 D$	247 227
219	$4f 5s^2 5p^5(^3F) 6s^2 F_{5/2}$	0.25 + $0.29 4f 5s^2 5p^5(^1D) 6s^2 D + 0.09 4f 5s^2 5p^5(^3F) 6s^4 F$	247 572
220	$4f 5s^2 5p^5(^3F) 5d^2 F_{5/2}$	$0.20 + 0.19 4f 5s^2 5p^5(^3G) 5d^2 F + 0.12 4f 5s^2 5p^5(^1D) 6s^2 D$	248 456
221	$4f 5s^2 5p^5(^3F) 5d^2 G_{7/2}$	$0.27 + 0.16 4f 5s^2 5p^5(^3D) 5d^2 G + 0.16 4f 5s^2 5p^5(^1D) 5d^2 G$	248 498
222	$4f 5s^2 5p^5(^3G) 5d^2 D_{3/2}$	$0.41 + 0.10 4f 5s^2 5p^5(^3F) 5d^2 D + 0.10 4f 5s^2 5p^5(^1G) 5d^2 D$	248 849
223	$4f 5s^2 5p^5(^3F) 5d^2 G_{9/2}$	$0.31 + 0.22 4f 5s^2 5p^5(^3D) 5d^2 G + 0.09 4f 5s^2 5p^5(^1F) 5d^2 G$	249 971
224	$4f 5s^2 5p^5(^3F) 5d^2 F_{7/2}$	$0.28 + 0.23 4f 5s^2 5p^5(^3G) 5d^2 F + 0.10 4f 5s^2 5p^5(^1G) 5d^2 F$	250 704
225	$4f 5s^2 5p^5(^3G) 5d^2 D_{5/2}$	$0.38 + 0.19 4f 5s^2 5p^5(^1G) 5d^2 D + 0.14 4f 5s^2 5p^5(^3F) 5d^2 D$	250 937

Table A.2. Comparison of computed wavelengths λ (in Å) and E1 transition probabilities A (in s^{-1}) in Ce IV with results from (Reader & Wyart 2009), (Carvajal Gallego et al. 2021), and (Savukov et al. 2003). Transition rates are given in the Babushkin gauge. dT is the accuracy indicator. The level numbers in the first and second columns match the ordering of the levels in Table A.1. ‘B/C’ in the (Carvajal Gallego et al. 2021) column means the Babushkin over Coulomb gauges ratio.

Odd level	Even level	GRASP2018			HULLAC		(Reader & Wyart 2009)		(Carvajal Gallego et al. 2021)		(Savukov et al. 2003)		
		λ	A	dT	λ	A	λ	A	λ	A	B/C	λ	A
1	219	403.92	3.61E+10	0.21523	418.66	3.19E+09	426.811	5.05E+09					
1	218	404.49	1.98E+10	0.20134	419.62	1.86E+09	427.385	7.70E+09					
1	217	405.27	6.23E+07	0.27270	423.30	7.20E+07	430.281	4.95E+07					
2	219	407.30	5.24E+07	0.26433	422.34	1.69E+07	430.954	5.82E+08					
1	214	410.22	1.32E+07	0.12091	426.61	6.33E+06	433.503	1.53E+02					
2	217	408.67	9.50E+09	0.20980	427.06	5.91E+09	434.495	7.99E+09					
2	216	410.65	4.42E+09	0.18501	430.22	2.72E+09	436.017	7.92E+09					
1	225	398.51	4.58E+08	0.14407	395.82	4.34E+09	436.288	1.98E+09					
2	214	413.70	3.47E+09	0.20869	430.43	1.75E+09	437.776	1.83E+10					
1	213	413.41	3.87E+09	0.16868	433.43	3.18E+09	438.823	9.23E+09					
1	222	401.85	5.70E+10	0.19601	399.56	1.32E+11	439.134	5.43E+10					
1	212	415.66	3.36E+09	0.20076	433.72	2.78E+09	439.650	3.27E+09					
2	225	401.79	7.15E+10	0.19821	399.11	1.28E+11	440.621	5.12E+10					
1	204	443.53	1.61E+08	0.05210	432.12	2.92E+08	440.975	7.78E+09					
2	205	446.94	3.12E+08	0.34304	436.17	9.01E+08	444.453	3.92E+10					
1	224	398.88	3.87E+07	0.79015	404.55	1.22E+10	444.605	2.69E+08					
2	204	447.60	4.79E+06	0.10003	436.04	3.53E+07	445.398	3.23E+09					
1	220	402.49	4.09E+10	0.22786	407.08	1.15E+11	446.318	7.18E+10					
1	221	402.42	6.96E+10	0.30668	407.20	1.07E+11	446.540	6.66E+10					
2	223	403.36	6.91E+10	0.31282	406.08	1.18E+11	448.669	3.48E+10					
2	224	402.17	7.33E+10	0.23292	407.98	1.08E+11	449.100	7.34E+10					
1	197	450.55	2.96E+06	0.32411	437.41	2.25E+08	449.280	3.75E+09					

Table A.2. Continued.

Odd level	Even level	GRASP2018			HULLAC		(Reader & Wyart 2009)		(Carvajal Gallego et al. 2021)		(Savukov et al. 2003)		
		λ	A	dT	λ	A	λ	A	λ	A	B/C	λ	A
2	221	405.77	1.09E+08	0.18677	410.69	1.27E+10	451.078	2.38E+09					
1	195	451.54	4.72E+08	0.21891	438.16	3.11E+09	451.138	2.53E+10					
2	197	454.75	6.04E+08	0.23896	441.43	1.95E+09	453.874	1.21E+10					
1	210	437.55	1.08E+09	0.20094	458.58	7.79E+08	465.911	9.90E+08					
1	209	439.54	5.47E+08	0.21120	460.91	3.04E+08	467.975	3.05E+08					
2	210	441.52	2.08E+09	0.22412	463.00	2.03E+09	470.852	2.35E+09					
1	207	441.35	4.32E+07	0.24841	465.64	2.76E+07	471.296	7.49E+07					
1	202	445.51	4.75E+08	0.34522	464.23	8.66E+08	475.345	1.73E+09					
2	207	445.39	2.45E+09	0.22026	470.19	1.97E+09	476.350	2.75E+09					
2	206	446.49	1.28E+09	0.10556	472.53	3.26E+09	478.080	1.20E+09					
1	198	449.15	2.81E+09	0.15214	474.79	2.64E+09	480.579	2.55E+09					
1	194	452.29	1.59E+09	0.21076	477.31	1.23E+09	481.454	1.43E+09					
1	190	457.84	7.61E+08	0.22334	481.95	1.11E+09	484.998	1.40E+09					
2	201	450.10	1.57E+09	0.22427	470.16	6.79E+08	485.361	4.00E+09					
2	198	453.33	2.07E+08	0.17745	479.53	3.09E+08	485.837	3.04E+08					
2	194	456.53	4.30E+07	0.16976	482.10	8.14E+07	486.729	3.52E+08					
1	184	460.11	1.71E+07	0.19526	488.68	1.60E+08	488.793	1.29E+09					
1	187	458.41	2.40E+09	0.18092	486.80	1.62E+09	489.853	1.56E+09					
2	190	462.18	2.84E+09	0.24404	486.83	2.49E+09	490.354	2.03E+09					
1	191	456.97	1.97E+06	0.72037	482.19	3.68E+06	491.233	1.49E+08					
1	185	459.68	1.39E+08	0.18782	484.37	2.40E+08	492.183	4.85E+08					
2	189	462.32	2.95E+09	0.14399	491.38	2.34E+09	493.854	2.39E+09					
2	184	464.50	4.36E+08	0.21381	493.71	1.43E+08	494.233	1.28E+08					
1	183	460.58	5.52E+08	0.19620	489.67	7.70E+08	495.174	6.94E+07					
2	187	462.77	1.28E+08	0.26917	491.78	3.13E+08	495.317	2.30E+08					
2	191	461.30	4.00E+07	0.12743	487.08	1.27E+08	496.730	8.39E+08					
1	169	469.29	2.46E+09	0.24445	496.39	1.71E+09	497.343	2.00E+09					
2	185	464.05	3.75E+06	0.15540	489.30	2.57E+08	497.699	3.00E+08					
2	180	466.06	1.22E+08	0.31695	498.46	2.75E+08	498.455	1.60E+08					
1	173	465.58	2.11E+08	0.29046	486.12	4.78E+08	499.581	2.90E+09					
1	159	472.94	1.50E+06	0.40269	501.32	6.73E+07	500.328	4.83E+08					
2	183	464.97	1.97E+08	0.23049	494.71	3.87E+08	500.765	2.39E+08					
2	176	469.01	2.63E+07	0.06322	494.53	3.35E+07	503.720	1.28E+08					
1	167	470.14	5.41E+08	0.25800	495.48	1.66E+08	505.262	1.27E+07					
1	164	470.47	1.14E+08	0.30343	497.72	1.48E+08	505.850	1.17E+08					
2	159	477.58	3.33E+06	0.57553	506.60	1.18E+08	506.029	1.36E+08					
1	153	478.69	6.62E+08	0.23321	508.57	8.20E+08	507.755	4.08E+08					
1	160	472.84	3.71E+08	0.20573	497.51	7.56E+08	508.501	1.44E+09					
2	167	474.73	2.62E+08	0.16552	500.64	1.62E+07	511.079	4.95E+07					
1	155	477.19	6.99E+08	0.40331	505.45	2.18E+08	511.079	3.51E+08					
2	165	475.00	2.34E+08	0.40324	509.00	1.88E+08	511.329	2.29E+08					
2	164	475.06	1.63E+08	0.31847	502.93	6.07E+07	511.680	1.79E+08					
1	151	479.66	4.24E+08	0.15685	507.10	6.19E+08	514.348	1.07E+09					
2	160	477.47	1.14E+09	0.22738	502.71	1.06E+09	514.389	1.58E+09					
2	157	479.04	8.09E+06	0.24121	511.75	1.17E+08	515.183	3.62E+07					
2	155	481.91	6.39E+06	0.41645	510.83	3.64E+05	517.029	1.05E+07					
1	149	482.85	4.44E+07	0.25166	510.00	5.70E+08	518.919	1.43E+08					
1	147	483.35	2.05E+09	0.20933	507.76	9.21E+08	520.896	2.98E+09					
1	146	484.58	1.28E+08	0.33000	519.71	2.34E+08	521.907	2.41E+08					
2	152	483.49	2.08E+08	0.37106	518.08	3.10E+07	522.650	3.83E+04					
2	149	487.68	1.04E+09	0.17899	515.47	4.68E+08	525.056	1.64E+09					
2	146	489.45	1.18E+08	0.20748	525.40	4.65E+08	528.115	2.96E+08					
1	144	488.95	2.08E+07	0.51226	521.98	8.79E+07	528.707	7.15E+07					
2	148	488.00	1.27E+09	0.35966	521.21	1.29E+09	529.444	2.56E+09					
1	132	496.68	6.61E+08	0.24286	531.17	8.78E+08	533.056	4.53E+08					
1	139	493.74	1.12E+09	0.35348	529.03	1.01E+09	534.345	2.24E+09					
2	144	493.91	1.53E+09	0.26627	527.72	1.06E+09	535.084	2.19E+09					
2	141	497.12	2.33E+08	0.35226	539.16	3.64E+08	536.832	3.18E+08					
1	130	499.86	8.72E+08	0.24674	528.25	1.87E+08	539.040	2.43E+09					
2	132	501.79	1.83E+07	0.48634	537.11	1.08E+08	539.532	3.63E+07					
2	139	498.80	1.31E+04	0.67350	534.92	7.88E+07	540.855	4.98E+08					
2	137	499.61	1.36E+08	0.35039	530.32	5.04E+07	541.645	5.62E+08					
1	126	503.66	2.13E+05	0.70578	533.63	2.61E+07	542.600	5.05E+07					
1	127	503.57	3.94E+08	0.38508	539.08	1.87E+08	545.375	5.00E+08					
2	130	505.04	6.21E+07	0.14652	534.12	7.30E+06	545.664	1.15E+08					
1	121	507.66	6.07E+07	0.34712	538.06	1.35E+08	545.868	1.85E+08					
2	127	508.83	1.36E+08	0.26163	545.20	6.74E+07	552.150	9.75E+07					
2	121	513.01	1.35E+06	0.99178	544.15	1.10E+08	552.665	2.20E+08					
1	117	510.31	4.93E+07	0.26406	547.11	2.31E+08	553.748	1.95E+08					
1	114	514.67	5.15E+04	0.76338	553.13	1.07E+08	555.133	1.90E+06					
1	103	521.11	1.33E+07	0.53916	556.84	1.13E+07	557.394	1.19E+07					
1	36	569.82	5.61E+07	0.37347	545.07	9.38E+07	558.932	2.68E+08					
2	117	515.71	7.74E+07	0.17793	553.41	4.25E+07	560.742	1.39E+08					

Table A.2. Continued.

Odd level	Even level	GRASP2018			HULLAC		(Reader & Wyart 2009)		(Carvajal Gallego et al. 2021)			(Savukov et al. 2003)	
		λ	A	dT	λ	A	λ	A	λ	A	B/C	λ	A
2	114	520.17	1.01E+07	0.47377	559.58	5.01E+06	562.168	9.73E+07					
1	105	519.54	1.59E+08	0.40320	557.35	2.16E+07	562.501	8.69E+07					
1	39	567.42	2.37E+06	0.41850	545.11	1.77E+07	564.338	2.02E+07					
2	113	520.94	1.54E+07	0.31179	557.36	5.93E+05	565.209	1.20E+07					
1	94	527.43	3.63E+07	0.12014	564.74	6.46E+07	569.004	3.73E+08					
2	105	525.14	3.61E+07	0.34383	563.89	3.90E+07	569.719	3.34E+04					
1	96	526.87	3.87E+07	0.38188	571.52	7.84E+07	571.004	8.69E+07					
2	39	574.11	9.45E+07	0.33838	551.37	1.09E+07	571.605	2.78E+08					
2	102	528.03	7.80E+07	0.48413	568.36	2.16E+07	572.532	1.26E+07					
2	100	528.73	1.56E+08	0.46975	570.96	7.71E+07	573.279	1.41E+08					
1	90	532.59	1.12E+07	0.09443	572.61	3.91E+06	573.566	3.08E+07					
1	89	533.69	4.13E+07	0.37008	577.50	4.35E+07	575.051	3.80E+05					
1	86	534.56	1.85E+08	0.25451	577.38	2.00E+08	577.209	3.40E+08					
1	83	536.88	1.79E+07	0.16214	574.33	1.06E+07	578.068	8.20E+07					
2	96	532.63	5.02E+07	0.26301	578.41	4.40E+07	578.444	9.25E+07					
1	88	534.00	2.25E+06	0.20043	576.70	4.06E+05	578.504	1.65E+06					
2	90	538.48	1.42E+08	0.25515	579.52	1.26E+08	581.073	2.63E+08					
1	84	536.22	5.23E+05	0.83134	583.29	2.98E+06	582.216	1.85E+04					
1	74	542.84	4.58E+07	0.33068	585.65	5.26E+07	583.971	6.53E+07					
1	75	542.46	2.68E+07	0.21006	585.76	6.73E+07	584.166	5.32E+07					
2	91	538.38	1.41E+04	0.95896	586.43	2.04E+07	584.625	1.87E+07					
2	86	540.49	1.48E+06	0.79282	584.40	3.48E+07	584.812	1.24E+05					
1	80	540.76	7.02E+06	0.44933	585.11	1.66E+06	585.100	6.41E+05					
2	88	539.92	9.09E+07	0.15096	583.71	6.17E+07	586.143	2.71E+08					
1	62	547.93	6.09E+06	0.16648	589.41	7.00E+06	589.166	1.04E+07					
1	69	544.57	1.93E+06	0.12517	592.15	1.86E+06	589.521	2.34E+06					
2	84	542.19	4.73E+07	0.33685	590.46	5.38E+07	589.951	5.01E+07					
2	75	548.57	1.02E+06	0.36298	592.99	1.75E+07	591.955	7.40E+06					
2	80	546.83	1.65E+04	0.56590	592.32	6.79E+07	592.915	8.48E+05					
2	81	545.12	1.46E+06	0.52598	591.39	1.36E+07	593.027	7.14E+06					
1	60	550.46	4.73E+06	0.24696	594.63	2.36E+07	593.447	9.58E+06					
1	55	554.38	7.04E+06	0.18398	598.85	7.47E+06	596.831	1.88E+07					
2	62	554.17	1.09E+07	0.12158	596.73	1.99E+07	597.090	3.82E+07					
2	69	550.72	4.39E+07	0.19648	599.54	7.35E+07	597.460	7.56E+07					
1	53	558.36	1.46E+06	0.05668	603.44	6.83E+06	601.448	4.85E+06					
1	54	557.16	2.15E+06	0.13828	609.87	3.54E+06	603.183	6.24E+06					
2	55	560.76	7.08E+05	0.38514	606.41	1.34E+06	604.964	1.65E+05					
1	45	564.71	2.22E+05	0.46698	617.43	5.04E+04	610.375	9.49E+05					
1	43	566.52	9.13E+07	0.08765	617.23	8.68E+07	610.472	1.67E+08					
2	54	563.61	5.76E+07	0.08174	617.71	5.94E+07	611.488	8.18E+07					
1	37	568.89	8.52E+06	0.15829	622.85	3.39E+07	613.145	6.68E+06					
1	32	574.02	1.28E+07	0.21517	624.01	2.39E+07	616.792	6.55E+07					
2	45	571.33	3.05E+07	0.09645	625.47	3.61E+07	618.884	4.98E+07					
2	43	573.19	2.00E+07	0.09381	625.26	2.48E+07	618.978	4.15E+07					
2	42	573.58	2.40E+04	0.86781	629.47	6.28E+06	620.298	4.25E+07					
2	34	580.10	1.89E+07	0.31792	643.74	2.22E+07	627.599	2.48E+07					
1	25	582.47	1.76E+07	0.34461	646.98	2.16E+07	629.405	2.46E+07					
2	25	589.52	1.82E+05	0.01116	655.81	1.48E+04	638.453	7.20E+05					
129	3	661.54	2.81E+08	0.01595	648.34	6.13E+08	671.033	4.14E+08					
128	4	672.73	1.62E+08	0.15092	650.11	4.41E+08	671.304	2.88E+08					
71	3	733.89	2.28E+09	0.00498	701.45	6.37E+09	741.808	4.05E+09					
73	4	746.25	2.77E+09	0.00171	713.75	6.67E+09	754.608	4.26E+09					
71	4	747.66	1.46E+08	0.01349	713.60	4.56E+08	755.760	2.75E+08					
129	5	886.64	2.19E+07	0.13499	900.21	8.44E+06	891.587	9.40E+04					
7	3	1269.95	1.27E+08	0.02689	1198.00	1.44E+08	1289.408	1.27E+08	1280.229	1.29E+08	6.80E-01	1289	1.22E+08
7	4	1311.77	1.11E+09	0.02155	1233.89	1.28E+09	1332.157	1.03E+09	1319.348	1.13E+09	6.83E-01	1334	1.06E+09
6	3	1348.52	1.16E+09	0.02286	1263.45	1.45E+09	1372.719	1.05E+09	1356.282	1.20E+09	6.62E-01	1371	1.11E+09
7	149	1239.01	3.84E+06	0.00509	1599.81	1.90E+07	1528.667	3.68E+07					
6	119	1337.35	2.33E+05	0.06265	1781.62	2.40E+07	1633.698	4.85E+07					
6	66	1635.86	5.08E+08	0.01754	1685.40	3.89E+08	1641.591	5.35E+08	1681.435	4.90E+08	8.26E-01		
7	130	1357.61	7.84E+03	0.65798	1794.24	9.00E+06	1717.489	6.57E+05					
7	119	1424.76	7.02E+05	0.20210	1930.34	4.38E+07	1769.788	7.90E+07					
6	36	1862.68	6.97E+08	0.02815	1844.45	1.19E+09	1775.304	7.75E+08					
7	66	1768.59	1.01E+09	0.01530	1817.90	7.90E+08	1779.060	8.35E+08	1815.113	9.75E+08	8.27E-01		
7	121	1416.71	1.19E+07	0.03397	1912.65	5.27E+08	1788.813	1.52E+08					
6	94	1475.11	2.25E+07	0.04000	2090.89	5.15E+07	1881.067	3.50E+08					
7	114	1472.69	2.71E+06	0.04402	2117.87	5.82E+07	1892.370	1.01E+08					
1	4	1993.49	2.28E+06	0.19572	1903.82	2.80E+06	1914.740	1.93E+06	1930.987	2.30E+06	5.94E-01	1994	4.56E+06
7	103	1526.71	9.97E+06	0.02736	2173.31	4.77E+07	1918.842	3.12E+08					
7	36	2036.72	1.18E+08	0.02557	2004.32	2.04E+08	1937.185	1.19E+08					
6	89	1525.19	1.29E+07	0.05191	2277.13	1.32E+05	1948.828	1.24E+08					
6	83	1551.55	5.54E+06	0.02525	2228.68	1.38E+07	1983.919	6.60E+05					
2	4	2078.55	4.12E+07	0.22325	1982.37	5.01E+07	2001.046	3.33E+07	2011.384	4.15E+07	5.62E-01	2086	8.41E+07

Table A.2. Continued.

Odd level	Even level	GRASP2018			HULLAC		(Reader & Wyart 2009)		(Carvajal Gallego et al. 2021)			(Savukov et al. 2003)	
		λ	A	dT	λ	A	λ	A	λ	A	B/C	λ	A
7	39	2006.45	1.02E+09	0.02705	2004.89	7.20E+08	2003.726	5.93E+08					
1	3	2098.51	4.06E+07	0.22504	1996.10	5.01E+07	2010.562	3.43E+07	2021.386	4.18E+07	5.76E-01	2102	8.56E+07
6	74	1602.32	6.27E+06	0.05356	2409.30	1.17E+06	2055.214	3.33E+06					
7	94	1582.18	4.38E+06	0.08474	2298.74	8.04E+06	2063.796	5.18E+07					
7	90	1629.61	7.34E+05	0.04017	2434.92	5.65E+06	2125.119	7.08E+06					
7	89	1639.94	1.55E+06	0.03773	2525.86	8.97E+04	2145.654	1.91E+07					
7	86	1648.16	2.95E+07	0.05247	2523.61	9.51E+06	2175.994	5.83E+07					
6	60	1670.65	1.82E+07	0.06000	2569.06	5.69E+05	2177.598	3.33E+06					
7	83	1670.46	1.59E+06	0.07980	2466.33	2.32E+06	2188.261	1.03E+04					
7	74	1729.46	8.50E+05	0.04183	2689.47	2.07E+05	2275.319	5.88E+05					
7	75	1725.70	1.72E+07	0.04651	2692.03	1.39E+06	2278.285	8.63E+06					
6	53	1745.57	1.03E+07	0.04910	2741.89	1.20E+05	2289.380	5.28E+05					
73	205	2402.26	5.03E+08	0.07554	2582.77	9.94E+08	2352.703	6.16E+08					
71	204	2406.58	5.44E+08	0.07084	2580.10	9.31E+08	2368.060	1.01E+09					
73	204	2421.36	2.31E+07	0.06356	2578.16	3.48E+07	2379.435	3.53E+07					
7	60	1809.32	2.32E+06	0.02419	2890.09	1.61E+05	2426.288	7.75E+05					
7	5	2477.36	3.99E+08	0.05400	2480.32	4.93E+08	2457.600	4.70E+08	2409.000	4.35E+08	9.04E-01	2465	3.95E+08
73	223	1519.66	6.24E+03	0.99371	1795.00	6.19E+07	2475.908	5.89E+08					
71	221	1548.34	1.07E+05	0.14094	1889.74	4.85E+07	2537.880	9.15E+07					
73	197	2646.57	1.94E+07	0.28284	2778.63	2.75E+07	2643.099	3.27E+07					
6	5	2795.03	2.78E+08	0.05605	2778.32	3.57E+08	2779.075	3.25E+08	2693.167	3.14E+08	9.23E-01	2785	2.72E+08
7	32	2091.45	9.03E+06	0.02582	3747.56	2.15E+04	2870.443	4.93E+04					
128	219	2050.83	6.81E+04	0.72959	3075.83	2.75E+06	3020.413	1.31E+06					