



UMONS - University of Mons Faculty of Sciences Atomic Physics and Astrophysics

Multi-platform computations of radiative properties and opacities in moderately-charged lanthanides in the context of early-phase kilonovae following neutron star mergers

A dissertation by Helena CARVAJAL GALLEGO

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Jury

Prof. P. Quinet (Université de Mons, Belgium, Supervisor)
Dr. P. Palmeri (Université de Mons, Belgium, Supervisor)
Prof. C. Semay (Université de Mons, Belgium, President)
Dr. E. Daubie (Université de Mons, Belgium, Secretary)
Dr. M-T Belmonte Sainz-Ezquerra (Universidad de Valladolid, Spain, Referee)
Dr. J-C. Pain (Université Paris-Saclay, CEA, France, Referee)

A mis estrellas, mi yayo, mi yaya,

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Contents

Int	Introduction					
1	Astr	Astrophysical context				
	1.1	Neutron stars			4	
	1.2	Binary systems of	f neutron stars		5	
	1.3	Origin of heavy el	lements		6	
	1.4	Heavy element op	pacities		9	
	1.5	Gravitational wave	e detectors		13	
	1.6	GW170817 event			16	
		1.6.1 Gravitation	onal signal		16	
		1.6.2 Electroma	agnetic counterpart		17	
		1.6.3 Analysis o	of the electromagnetic counterpart and production of lanthanides		19	
	1.7	Importance of ator	mic data in moderately-charged lanthanides atomic data		20	
2	The	oretical and compu	utational approaches		22	
	2.1	Pseudo-relativistic	c Hartree-Fock method and corrections related to the polarization of the	e atomic		
		core (HFR+CPOL			22	
		2.1.1 Basics prin	inciple of the HF method		23	
		212 Relativisti	ic corrections (HFR method)		25	
		2.1.2 Retaining	prization corrections (HER+CPOL method)		26	
		2.1.5 Core point 2.1.4 The matrix	x method		20	
		2.1.4 The main	arths transition probabilities and oscillator strengths		28	
		2.1.5 Enterstreng	code procedure		30	
	22	Multi-Configuration	onal Dirac-Hartree-Fock method (MCDHF)		31	
	2.2	221 Relativisti	ic quantum mechanics: the hydrogen atom problem		31	
		2.2.1 Relativisti	voinle of the MCDHE method		31	
		2.2.2 Dasic print	algorithmetrics corrections		27	
		2.2.5 Qualitum e			20	
		2.2.4 Transmon	1 probabilities		20 40	
	2.2	2.2.5 GRASP2018 code procedure		40		
	2.3	Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT)			42	
		2.3.1 Configurat			42	
		2.3.2 Exact Han			43	
		2.3.3 Many-bod	ly perturbation theory		44	
		2.3.4 Emu CI .	· · · · · · · · · · · · · · · · · · ·		48	
		2.3.5 AMBiT pa	ackage		49	
3	Ator	Atomic data obtained from pseudo- and fully-relativistic computational methods				
	3.1	Atomic structures	for moderately-charged lanthanides from $Z = 57$ to 71		51	
		3.1.1 La V–X io	ons		51	
		3.1.2 Ce V–X io	ons		61	
		3.1.3 Pr V–X ion	ons		70	
		3.1.4 Nd V-X io	ons		76	
		3.1.5 Pm V–X io	ons		81	
		3.1.6 Sm V–X io	ons		85	
		3.1.7 Eu V–VII	to Lu V–VII		89	
	3.2	Ground states for l	La V–X to Sm V–X and Eu V–VII to Lu V–VII		97	
	5.2	Ground states for I	La $v - \Lambda$ to SIII $v - \Lambda$ and Eu $v - V$ II to Lu $v - V$ II			

4	Astrophysical opacity calculations using pseudo- and fully-relativistic atomic data	101				
	4.1 Expansion formalism	101				
	4.2 Astrophysical conditions	103				
	4.3 Impact of using realistic partition functions in Sobolev optical depth	106				
	4.4 Impact of atomic computations on the opacities	107				
	4.5 Expansion opacities for La V–VII to Lu V–VII	110				
	4.6 Line-binned opacities	112				
	4.7 Planck mean opacities	115				
5	Atomic data and astrophysical opacities obtained from the Statistical Resolved Transition Array					
	(RTA) method	¹¹⁷				
	5.1 <i>Ab initio</i> method	118				
	5.1.1 Energy levels	119				
	5.1.2 Transition wavelengths	120				
	5.1.3 Oscillator strengths	120				
	5.2 <i>A posteriori</i> method	121				
	5.3 Sm VIII and Eu VI	122				
	5.4 Dy VIII	128				
Conclusions and prospects 132						
Ap	Appendices					
A	Comparison of the radiative parameters for La V-X ions	142				
B	Comparison of the radiative parameters for Ce V-X ions	163				
С	Comparison of the radiative parameters for Pr V					
D	Comparison of the radiative parameters for Nd V					
Е	Comparison of the radiative parameters for Yb V					
F	Comparison of the radiative parameters for Lu V					

Introduction

One of the great unresolved questions in physics is "How were the heavy elements between iron and uranium formed?". While it is well known that light elements (Z < 26) of the periodic table up to and including iron are synthesized by nuclear fusion within stars, the nucleosynthesis of the heavier elements (Z > 26) remains a great *enigma*. Indeed, the production of the latter requires very specific physical conditions for neutron capture by atomic nuclei, as nuclear fusion changes from exothermic to endothermic beyond iron (Ryan and Norton, 2010). Consequently, all elements heavier than iron (Z > 26) are the result of neutron addition, transforming already massive atomic nuclei into even more massive elements. Supernova explosions and the extreme conditions (high pressure and very high temperature) they generate have been considered the main sources of heavy elements production for sixty years (Cameron, 1957). These conditions give rise to numerous nuclear reactions, with an abundant production of neutrons whose rapid flux enables atomic nuclei to transmute into elements heavier than the previous ones. This fast neutron capture is the nucleosynthesis process well known as the r-process (r for rapid), and its role in the formation of the heavy elements of the periodic table has been repeatedly described in the scientific literature (Rauscher, 2020; Shaviv, 2012; Cowan et al., 2021). However, the development of increasingly advanced numerical simulations for supernovae has revealed that the conditions necessary for the formation of heavy elements do not last long enough in those explosions to explain the abundances of elements heavier than iron observed in the Universe (Cowan et al., 2021). In the late 80s, some researchers suggested that neutron star merger could be another interesting candidate to be the site of production of heavy elements (Eichler et al., 1989). However it was felt at that time that this type of collision was too rare to contribute significantly, although successive theoretical modelings confirmed this hypothesis, as indicated by hydrodynamical simulations (Goriely et al., 2011).

Neutron stars can evolve in binary systems. Each neutron star approaches each other losing energy until it merges with the other one. This binary system of neutron stars produces gravitational waves. The latter have fascinated scientists for decades. These waves were theoretically predicted by the physicist Albert Einstein in 1916 but were only observed for the first time almost a century later, in 2015, with the detection of a black hole merger (GW150914 event, Abbott et al. 2016). These oscillations were detected by the LIGO and Virgo Collaboration with the LIGO interferometers which are Michelson interferometers located at Hanford (Washington) and Livingston (Louisiana) in the United States. Virgo interferometer located near Pisa in Italy was not operating at that time since it was shut down for an equipment upgrade and could therefore not confirm the signal recorded by LIGO interferometers (Castelvecchi and Witze, 2016). Nevertheless, such gravitational waves recorded by LIGO interferometers made it possible to characterize and partially localize the binary system before it collapsed. Unfortunately, for this event, no electromagnetic counterpart was observed by the Fermi, INTEGRAL and Swift space telescopes (Evans et al., 2016).

On August 17, 2017, gravitational waves emitted by a neutron star merger (NSM) were detected for the first time by the above-mentioned interferometers (Abbott, 2017). This event, named GW170817, was followed by a short gamma-ray burst detected 1.7 seconds later by the Fermi and INTEGRAL space telescopes (Abbott et al., 2017). This collision also produced an electromagnetic signal powered by the ejection of hot and radioactive matter, known as a kilonova (thousand times brighter than a nova) and named AT2017gfo in the case of the abovementioned NSM event. The latter was recorded by several tens of telescopes, operating in the infrared, the visible, the ultraviolet and the X-ray wavelength ranges. The spectral analysis of AT2017gfo revealed the presence of elements heavier than iron (Kasen et al., 2017). The total quantity of heavy elements produced by this coalescence was estimated to be 16 000 times the mass of the Earth, opening up a robust path towards the conviction that a large proportion of the elements created by the r-process originated in neutron star mergers (Berger, 2017). The matter ejected during such event is characterized by a substantial opacity. The latter is essentially due to the superposition of millions of spectral lines belonging to ions of the lanthanide group (Z = 57-71) and actinide group (Z = 89-103) whose atomic structures consist in the progressive filling of the 4f and 5f subshells, giving rise to complex electronic configurations with a huge number of closely spaced energy levels. In other words, lanthanide and actinide ions significantly contribute to the kilonova ejecta opacity. Combining the detection of gravitational and electromagnetic waves to characterize the same celestial object allows the birth of a new physics, the so-called *multi-messenger* astronomy. By considering complementary physical phenomena from different disciplines, it is feasible to localize as accurately as possible the position of NSM to quickly observe the electromagnetic counterpart and better understand the formation of heavy elements.

Unfortunately, atomic data for moderately-charged lanthanides and actinides are still too incomplete, both in quantity and quality, to accurately model kilonovae, especially with regard to the opacity and the light curve, *i.e* the evolution of luminosity as a function of time. However, in the purpose of interpreting and modeling kilonova spectra, it is imperative to have an accurate understanding of the radiative parameters that characterize these elements notably for lanthanides to which the present work is devoted. Although the determination of such parameters has already been the subject of various studies over the recent years, the latter only concern the first ionization degrees (up to 3+) and are therefore limited to the analysis of kilonovae in a temperature range below 20 000 K. To extend the modeling of this type of celestial object to higher temperatures, corresponding to the early phase of kilonovae (less than a day post-merger), it is essential to know the radiative parameters of lanthanide ions in higher charge stages for which only few studies have been conducted so far. This work aims to make a significant contribution in this field as it consists in a detailed study of the radiative processes characterizing moderatelycharged lanthanide ions (from 4+ to 9+) and to deduce the corresponding astrophysical opacities for typical early-phase kilonova ejecta conditions 0.1 day after the merger. As there is almost no experimental data available for these ions, our calculations are based on a multi-platform approach involving different independent theoretical methods, namely the pseudo-relativistic Hartree-Fock (HFR) (Cowan, 1981), the fully-relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) (Grant, 2007) and the Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT) (Dzuba et al., 1996) methods. Due to the absence of sufficient experimental data, this approach is the only way to estimate the accuracy of the results obtained through systematic comparisons between distinct computational procedures. Nevertheless, some ions are difficult to treat with these computational methods due to the enormous size of their corresponding Hamiltonian matrices. In that case, the so-called Resolved Transition Array (RTA) (Bauche et al., 2015) statistical approach is used to simulate atomic data and to compute opacities.

In the first chapter of this work, we detail the astrophysical context, highlighting the formation of neutron stars and the evolution of neutron star binary systems. We also explain the *r*-process allowing the formation of heavy elements and detail the different types of ejecta formed after a NSM. The behaviour of a kilonova throught the time is also shown. A brief explanation of gravitational wave detectors is given, followed by a description of the GW170817 event. To conclude this chapter, we explain the importance of calculating atomic parameters in moderately-charged lanthanides and we detail the atomic data already available to analyze our atomic results and opacities computed for lanthanide ions.

In the second chapter, we present the theoretical concepts and computational methods used to model the atomic structures and radiative data of moderately-charged lanthanide ions. The first method described is the pseudo-relativistic Hartree-Fock (HFR) method implemented in Cowan's code. Then, we detail theoretical background of the fully-relativistic Multi-Configuration Dirac-Hartree-Fock approach (MCDHF) and also describe the GRASP2018 package which implement such method. Finally, the Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT) method executed by AMBiT is also explained.

Chapter 3 and 4 present the atomic data and astrophysical opacities obtained using different computational methods based on the above-mentioned theoretical strategies. In this former, we first detail the atomic calculations performed for La V–X to Sm V–X ions. Then, we show how the atomic data for Eu V–VII to Lu V–VII ions are computed. A comprehensive study and comparison is also carried out in order to determine ground levels of moderately-charged lanthanide ions. After that, in Chapter 4, we explain the expansion formalism useful to compute expansion opacities in this work. The influence of some parameters such as cancellation factor (CF), scaling factor (SF), cut-off on oscillator strengths and the use of realistic partition functions instead of approximating the latter by only considering the statistical weight of the ground level on the computed opacity is also described. The line-binned formalism is also investigated for a specific lanthanide, namely Sm ions in order to make a comparison with the corresponding expansion opacities obtained with the expansion formalism. At the end of this chapter, we determine Planck mean opacities for moderately-charged lanthanide ions between 25 000 K and 40 000 K, to find out the opacities of which elements are dominant depending on the temperature.

The last chapter of this work focusses on the determination of simulated atomic data by using the Resolved Transition Array (RTA) approach. The latter is a statistical method that we used to calculate opacities for complex ions difficult to treat with the computational methods previously cited. Statistical distribution used to obtain energy levels, wavelengths and oscillator strengths through random draws are described in this chapter. Opacities calculated using HFR results and simulated atomic data are compared for Sm VIII and Eu VI before applying the statistical method to a complex ion difficult to treat with the Cowan's code, namely Dy VIII. Finally, we draw the general conclusions of our investigations and develop some interesting prospects.

Chapter 1

Astrophysical context

The first chapter aims to detail the main motivations of this PhD thesis from an astrophysical point of view. The first sections describe the formation of neutron stars and the evolution of neutron star binary systems. Then, the physical processes creating heavy elements that make up our universe are introduced and the different ejecta types involved in the merger of two neutron stars (NSM) are explained. In the following section, the concept of opacity is described and some examples are shown for heavy elements such as lanthanides (lowly- and moderately-charged). Subsequently, before relating the NSM event observed on August 17, 2017, detectors used to observe these gravitational waves (their improvements and the latest upcomings) are briefly presented. Finally, the last part of this chapter explains the importance of obtaining atomic data for the moderately-ionized lanthanides which are essential to model kilonova light curves.

1.1 Neutron stars

In the core of the stars, thermonuclear fusion reactions take place, ensuring the stability of the star. These reactions provide the required energy to the stars to counterbalance their own weight *via* radiation pressure, in order to assemble nucleons to form an atomic nucleus heavier than the initial one. If the nuclear binding energy per nucleon is higher in the formed nucleus, a release of energy occurs (exothermic reaction). In stars, such reactions happens up to 56 Ni. The latter is unstable and it decays into 56 Fe, which is stable. This process does not continue beyond iron because fusion reaction becomes endothermic (*i.e.* the reaction requires energy to happen). As no force can counterbalance the weight of the star at this point, there is a gravitational collapse of the star on itself giving rise to a supernova. The latter is extremely bright and lasts only a few days or few weeks.

Depending on the mass of the initial star, the star of mass M ($M > 8M_{\rm sol}$ where $M_{\rm sol} = 1.94 \times 10^{30}$ kg) has two possible *scenarii* after the supernova stage: either it becomes a neutron star ($8M_{\rm sol} > M > 25M_{\rm sol}$) or a black hole ($M > 25M_{\rm sol}$). If the initial star has a mass lower than eight solar masses then it will become a white dwarf (*i.e.* a celestial object of high density with a high surface temperature) (Pradhan and Nahar, 2011). In this work, only the neutron stars are of interest.

When the explosion occurs, the collapse only stops when the matter is very dense so that no nucleus can exist and the neutrons are separated by distances on the scale of a fermi (*i.e.* 10^{-15} m). Indeed, the Pauli principle, which describes that two particles cannot occupy the same space at

the same time t, must be respected. At this point, the strong interaction (responsible for the cohesion of the atomic nucleus) is dominant and causes a sufficient pressure to stop the collapse. There remains only a very dense core composed mainly of neutrons. This remaining star has a radius of a few tens of kilometers, while its mass is between 1.4 and 3.2 times the mass of the Sun. Neutron stars are the smallest and densest stars known to date.

A neutron star, whose existence was assumed in 1930 by the physicist Lev Landau (Yakovlev et al., 2013), was detected and observed for the first time in the 1960s by the physicist Jocelyn Bell (APS news, 2006), thanks to the pulses of radiation that such stars emit, as illustrated in Figure 1.1 (Thielmann et al., 2017). Indeed, when neutron stars are formed, they rotate on themselves at very high speed making their magnetic field amplified. Such stars behave like a giant magnet turning very quickly on themselves. As the magnetic pole axis is not in the same direction as the rotation axis, the radio emission is focused along the magnetic poles sweeping periodically a limited region. A radio pulse can only be detected when Earth occupies this specific region. Due to the detection of this pulse, such neutron star are called a *pulsar* (Blanchet et al., 2017). A neutron star can be also called a *magnetar*. Such as the pulsar, it turns rapidly around itself and have a magnetic field's intensity which is a 100 to 1000 times more powerful than pulsars.



Figure 1.1: Artist's view of relativistic jets emanating from a neutron star (https://www.skyatnightmagazine.com/space-science/what-is-a-pulsar-a-complete-guide-to-spinning-neutron-stars).

1.2 Binary systems of neutron stars

Some neutron stars evolve in binary systems. They revolve one around the other, as shown in Figure 1.2, and slowly approach each other while losing energy until they merge. This *scenario*, predicted theoretically, has been observed experimentally only few years ago. Binary systems of neutron stars produce gravitational waves (*i.e.* vibrations of space-time predicted by the general relativity). These waves have frequencies that are directly related to the orbital frequency, meaning the rate at which the two stars orbit each other. These waves propagate at the speed of light and are generated by the relativistic movements of large amounts of matter (Blanchet et al., 2017).

As shown in Figure 1.2, there are three phases when considering a binary system of neutron stars. First, the gravitational wave carries away part of the energy of the considered system,

causing the two celestial bodies to spiral towards each other. Secondly, stars get closer and at a certain time, they merge, as illustrated on the third Figure: this phenomenon is called a *coalescence*. When the latter happens, gravitational waves may reach the Earth and can be detected with suitable detectors. Finally, a relaxation phase can be detected in order to define the object resulting from the coalescence. In the case of neutron star mergers, the remaining object can be a stable neutron star, a massive long-lived neutron star (*i.e.* a neutron star with a mass greater than the maximum mass for a non-rotating neutron star and less than the maximum mass for a uniformly rotating star), a hypermassive neutron star (*i.e.* with a mass greater than the maximum mass of the binary system. The process is relatively long since it typically takes 10^8 years for the neutron star system to merge (Weinsberg and Huang, 2016).



Figure 1.2: Artist's view of the evolution of a binary system of neutron stars (http://public. virgo-gw.eu/the-gravitational-wave-universe/).

1.3 Origin of heavy elements

The synthesis of elements ranging from carbon to iron is well known. They are synthesized by nuclear fusion processes in stars. However, the nucleosynthesis of elements heavier than iron remains a great *enigma*. Their production requires very particular physical conditions allowing the capture of neutrons by the nuclei. Schramm and Symbalisty (1982) suggested that the physical conditions encountered during the collision of neutron stars could explain the origin of some heavy elements such as those illustrated in dark blue in Figure 1.3 including in particular lanthanides (Z = 57-71) (Crockett, 2018).



Figure 1.3: Heavy elements formed during the neutron stars merger illustrated in dark blue (Crockett, 2018).

Two nuclear processes allow the formation of such heavy elements. First, the process of slow neutron capture, the *s*-process (*s* for *slow*), which consists of the neutron capture by atomic

elements known to date.

nuclei. This process is qualified as a slow process since it occurs over a few thousand years. Indeed, by capturing a neutron, the mass number, A, of an initial nucleus increases and the resulting nucleus becomes heavier. The latter remains stable for a long time (100 to 100 000 years) but becomes unstable at some point. By decaying *via* β -decay which converts a neutron into a proton, an electron and an anti-neutrino, the heavy nucleus becomes stable again and the neutron capture process can be renewed. This process typically appears in stars aged by a few million years appearing in the so-called asymptotic giant branch (AGB). Such stars create half of the elements heavier than iron (Cowan et al., 2021). However, this process takes a long

The other process called the *r*-process (*r* for *rapid*), is able to produce heavy nuclei faster than the previous one. This process of nucleosynthesis consists in neutron capture by atomic nuclei at high temperature and at high neutron flux. While a nucleus capture the neutron flux, it becomes unstable. This process is faster than the *s*-process since the β -decay does not have time to occur between each neutron capture. The nucleus is therefore filled with neutrons until it can no longer contain any more neutrons. Such a nucleus, which is thus unstable, can undergo two possible *scenarii*. It can either split into two lighter nuclei due to the presence of very energetic photons in the space, or it can become a stable heavy nucleus when one of these neutrons decays into a proton (in about 0.01 seconds) by β -decay (Crockett, 2018). These decays produce a large amount of energy and can lead to electromagnetic emissions. This entire process takes about 1 second in contrast to a few thousand years for the *s*-process (Cowan et al., 2021).

time to create a heavy nucleus and is therefore too long to allow the synthesis of all the heavy

During the neutron star coalescence, a certain amount of matter is emitted at very high speed in all directions (Kasen et al., 2013). Neutron star mergers has three types of ejecta (Martin et al., 2017). According to hydrodynamics simulations, the first ejection called dynamical ejecta, occurring 1 ms after coalescence, has predicted masses of the order of 10^{-3} to 10^{-2} solar mass and a velocity from 0.1c to 0.3c (where c is the speed of light). This ejection, characterized by the compactness and by the mass of the neutron star, consists in the expulsion of the star's surface layers (Kasen et al., 2017). Moreover, this ejecta has two components. A cold component coming from tidal interactions during the merger, ejecting matter along the equatorial plane and a hot component coming from the matter compressed by hydrodynamic forces at the contact interface, ejecting matter along the polar directions. The outermost layers of the polar ejecta may contain free neutrons, whose decay causes a UV emission during a few hours after the merger. In the equatorial plane, the electron fraction (Y_e) is relatively small (*i.e.* $Y_e < 0.1$). It results in a dominant r-process producing heavy elements (with mass number A exceeding 130), e.g. lanthanides and actinides (Tanvir et al., 2017). In the polar directions, the electron fraction is much higher (*i.e.* $Y_e > 0.25$) and consequently *r*-process does not occur. Therefore, elements which are characterized by a mass number less than 130 are then formed (Cowan et al., 2021).

During the coalescence of such stars, matter gathers around the resulting central object and forms an accretion disk of about 0.01 to 0.3 solar masses (Metzger, 2017). After formation of the latter, two other ejecta can be highlighted. One of them is formed about 100 ms after coalescence and comes from a neutrino winds expulsion along the polar directions. It has the same mass as the first ejection but a velocity of 0.08c (Cowan et al., 2021). This expulsion contains about 5% of the mass of the accretion disk. The formation of the second ejecta occurs one second after the stars merge. Some of the ejected material from the viscous flow of the accretion disk is expelled isotropically. This ejecta has a mass about 10^{-2} to 10^{-1} solar mass

and a velocity ranging from 0.05c to 0.1c. The latter carries away about 40% of the accretion disk mass. Since the electron fraction is high (*i.e.* Y_e > 0.25) in these two ejecta, elements with A < 130 can also be created (Cowan et al., 2021).

The amount of matter ejected during the coalescence can be determined by numerical simulations. For that purpose, it is necessary to use simulations that solve both the Einstein equations (making the link between curvature of space-time, mass and energy densities) and the relativistic hydrodynamics equations (which describe dense matter as present in neutron stars). These simulations show that the amount of ejected matter depends on many parameters, such as the masses of the neutron stars, their sizes and the way the matter is gravitationally bound in these stars (Coté et al., 2019). The amount of lanthanides produced thus depends on the amount of mass ejected by the binary system.

The coalescence phenomenon of two neutron stars is followed by an electromagnetic counterpart (*i.e.* other types of emission from the same object). A short-lived gamma-ray burst (a narrow, symmetric beam of matter reaching relativistic speeds) occurs. This burst proves that nucleosynthesis including radioactive heavy nuclei takes place in a neutron star merger (Tanaka and Hotokezaka, 2013). In addition, an Ultraviolet-Optical-Infrared (UVOIR) emission, called kilonova, is emitted, which comes from the decay of these radioactive heavy elements created by *r*-process during the coalescence of neutron stars. As shown in Figure 1.4, the blue component of the kilonova comes from the production of the light elements (*i.e.* $28 \le Z \le 57$) and has a maximum in the optical/blue range whereas the red component comes from the formation of the heavy elements such as lanthanides or actinides and has a maximum in the optical/red range. The black curve represents the summation of both components. This one moves towards longer wavelengths (*i.e.* infrared) and its intensity decreases with time. Such UVOIR emission is called kilonova because it reaches a much lower maximum luminosity compared to a supernova but it remains a thousand times brighter than a nova (explosion phenomenon on the surface of a white dwarf) (Metzger, 2010).



Figure 1.4: Kilonova spectrum model representing the components formed by light r-process (blue) and the components formed by heavy r-process (red) and the black curve being the sum of both contributions (Kasen et al., 2017).

1.4 Heavy element opacities

The production of lanthanides in the equatorial plane within the *dynamical ejecta* is characterized by a very high opacity. This is due to the numerous spectral lines originating from the complex atomic structure of lanthanides characterized by configurations with an open 4f subshell (Kasen et al., 2013). To understand the opacity produced by these elements, the optical depth τ has to be defined. This dimensionless quantity is such that

$$I = I_0 e^{-\tau}, \tag{1.4.1}$$

where I is the radiation propagating through matter and I_0 is the incident radiation. The exponential factor is known as the probability that the radiation escapes from the material:

$$P(\tau) = e^{-\tau}.$$
 (1.4.2)

As $0 \le P(\tau) \le 1$ thus $0 \le \tau \le \infty$. The medium is opaque when the optical depth tends to infinity and is transparent when it tends to zero. By convention, a medium is optically thin when $\tau < 1$ and optically thick when $\tau > 1$. The optical depth depends on the geometrical dimensions of the medium, but also on the quantity of matter passing through it, on its macroscopic states (temperature and density) and on its microscopic properties (absorption, emission and chemical composition). Therefore, the macroscopic bolometric opacity can be defined as a function of the dimensionless optical depth τ as

$$\tau = \int \rho \,\kappa \,\mathrm{d}s, \tag{1.4.3}$$

where the curvilinear integral relates to the geometrical path of the radiation and where ρ is the density (g cm⁻³). The macroscopic opacity κ is expressed in cm² g⁻¹ (CGS units). The opacity depends on the wavelength and on the frequency of the radiation and is known as the monochromatic opacity. The monochromatic microscopic opacity (cm⁻¹) is thus obtained by

$$\kappa_{\nu}^{\text{micro}} = \kappa_{\nu}^{\text{macro}} \rho. \tag{1.4.4}$$

It is no coincidence that the kilonova emission shown in Figure 1.4 is centered in the visible/infrared band, as this is one of the first spectral windows in which the emission due to the ejection of expanding fusion material becomes transparent. Figure 1.5 provides a semiquantitative illustration of the opacity of neutron star merger ejection as a function of photon energy. In the radio and far-infrared region, free-free transitions of the ionized gas are predominant. At near-infrared and visible frequencies, the dominant source of opacity is a dense window of bound-bound transitions. The magnitude of the effective continuum opacity is determined by the oscillator strengths and the spectral density of the absorbing lines, which depend on the composition of the ejecta. If the latter contains elements with relatively simple valence electron structures, such as iron, the resulting opacity is relatively low (dotted brown line). On the other hand, if the ejecta contains a fraction of elements with partially filled 4f- or 5f-shells, such as those of the lanthanide and actinide groups, the opacity is higher. In the far UV and soft X-rays, bound-free transitions of the partially neutral ejecta dominate the opacity, whereas in the hard X-rays and γ -rays, it is electron scattering that provides significant opacity (Metzger, 2017).



Figure 1.5: Schematic illustration of neutron star merger ejection opacity as a function of photon energy (Metzger, 2017).

Depending on the heavy element considered, the opacity will be relatively different. In Figure 1.6, the Planck mean opacity is represented as a function of the wavelengths. The former is the average of the opacity over a wavelength range at a certain temperature and defined as

$$\kappa_{\text{Planck}} = \frac{\int_0^\infty B(\lambda, T)\kappa(\lambda) d\lambda}{\int_0^\infty B(\lambda, T) d\lambda} \quad \text{with} \quad B(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}, \tag{1.4.5}$$

where $B(\lambda, T)$ is the Planck black-body function. In this Figure, we can notice that, when the temperature increases, the excited levels become more populated and the number of optically thick absorption lines increases. The Planck mean opacity increases with temperature until the gas becomes hot enough to get ionized. This leads to multiple maxima in the opacity curve, each one occurring around the transition temperatures of the different ionization states. At sufficiently low temperature, when the element becomes neutral, opacity fade abruptly and decrease exponentially with decreasing temperature. As it can be seen in this Figure, according to some calculations detailed by Kasen et al. (2013), the Planck mean opacity produced by the f-shell elements in such conditions ($\rho = 10^{-13}$ g cm⁻³, a time after the merger t = 1 day and $T < 20\,000$ K, known to be the conditions corresponding to the presence of lowly-ionized elements in the ejecta (Tanaka et al., 2020)) is 10 to 100 times higher depending on the temperature than opacity produced by d-shell or p-shell elements, e.g. iron or silicon. A notable characteristic of f-shell elements (as indicated by the blue curve) is their tendency to maintain high opacity at comparatively lower temperatures compared to the elements belonging to the d-shell or p-shell group (green and red curve). Indeed, the ionization potentials of lanthanides are generally about 30% lower than those of iron group elements (Kasen et al., 2013).



Figure 1.6: Planck mean opacities for three different elements. Calculations assume a density $\rho = 10^{-13} \text{ g cm}^{-3}$ and an elapsed time since ejection t = 1 day (Kasen et al., 2013).

It can also be noticed in Figure 1.7 that d-shell elements such as Os II and Fe II have smaller opacity compared to Nd II and Ce II, lanthanide ions, characterized by a partially filled f-shell. Another feature that can be seen from this Figure is that the opacity of such elements decrease much slower compared to opacity of d-shell elements. This is due to the high spectral density of lanthanides. This feature allows lanthanides to cover not only UV wavelengths but also the entire optical region of the spectrum.



Figure 1.7: Expansion opacity according to wavelength for different elements. Calculations assume a density $\rho = 10^{-13} \text{ g cm}^{-3}$ and an elapsed time since ejection t = 1 day (Kasen et al., 2013).

Depending on the lanthanide element considered and also on its ionization degree, the opacity will be different. For example, lanthanum (La) I–IV and lutetium (Lu) I–II ions have no electrons on the f-shell while Lu III–IV have 14 electrons on the f-shell, *i.e.* the maximum number of electrons that this subshell can contain. As they have an empty or a full f-subshell, these

elements will produce a lower opacity compared to the ones having a half-filled subshell, as the gadolinium (Gd) I–IV (*i.e.* 7 electrons on the f-shell). Figure 1.8 shows the Planck mean opacity computed with conditions such as $\rho = 10^{-13}$ g cm⁻³ and an elapsed time since ejection t = 1 day where lowly-ionized lanthanide elements (from I to IV) are expected to be formed. As an example, for T = 5000 K, where typically there are mainly singly ionized lanthanides (II spectra), Planck mean opacity for Pr, Nd and Pm (Z = 59, 60, and 61) are the highest among the others according to Tanaka et al. (2020) calculations. Opacity of such elements gradually decreases for higher charge states (III and IV) as less electrons occupy the 4f-shell.



Figure 1.8: Planck mean opacities for lowly-ionized lanthanides. Calculations assume a density $\rho = 10^{-13} \text{ g cm}^{-3}$ and an elapsed time since ejection t = 1 day (Tanaka et al., 2020).

The previous Figures only concern the lowly-ionized lanthanides for conditions encountered in the kilonova ejecta about 1 day post-merger such as $\rho = 10^{-13}$ g cm⁻³ and $T < 20\ 000$ K. If one wants to extend study to higher temperatures, it is essential to study moderately-ionized lanthanides (from V to X). The conditions to have such degree of ionization are encountered in early-phases kilonova, *i.e.* conditions such as $\rho = 10^{-10}$ g cm⁻³, a time after the merger t = 0.1day and $T > 20\ 000$ K. These conditions can be deduced from radiative transfer simulations (Banerjee et al., 2023). When considering such degrees of ionization, lanthanide ions can be characterized both by a half-filled p-shell and by a half-filled f-shell. An example can be seen on Figure 1.9 where Tb to Tm ions between VIII to X (corresponding to temperatures ranging between 60\ 000 K and 100\ 000 K) show the highest opacity (Banerjee et al., 2023).



Figure 1.9: Planck mean opacities for moderately-charged lanthanide ions. Calculations assume a density $\rho = 10^{-10} \text{ g cm}^{-3}$ and an elapsed time since ejection t = 0.1 day (Banerjee et al., 2023).

1.5 Gravitational wave detectors

Gravitational wave detection has predominantly been approached through two main methods. The first one is based on measuring the amplitude of oscillations of a resonant bar, where the oscillations originate from gravitational waves. In order to do that, the Allegro, Auriga, Explorer, Nautilus and Niobe detectors (Baggio et al., 2000) were built based on the works of Weber (1960). The second approach uses interferometry to detect variations in the space-time, which are sensed by freely falling masses. Since the 1980s, the latter has seemed to be the most promising technique to detect gravitational waves. During the passage of these waves, spacetime is distorted. Therefore, the distance between two objects will oscillate in a minimal way. Figure 1.10 explains the operation of a Michelson interferometer. The light from an ultrastable laser is split in two by a semi-reflective mirror (the beam splitter). Therefore, each of these beams travels a certain distance in the arms of the interferometer until it reaches a mirror that sends the light back to the beam splitter until it reaches the detector. At this point, both beams interfere. The intensity of the recombined laser beam depends on the length variations of one arm with respect to the other arm, *i.e.* on the variation of the path difference of the laser waves traveling through both arms of the interferometer. Its measurement carries the signature of the gravitational wave (Mours et al., 2017).



Figure 1.10: The Michelson interferometer (https://fr.wikipedia.org/wiki/ Interférométrie).

Several detectors based on a Michelson interferometry with km-long arms have been built namely LIGO, Virgo, GEO600 and KAGRA. The mirrors of the interferometer act as freefalling test masses. First, LIGO more particularly LIGO-Hanford and LIGO-Livingston located in the United States respectively in the Washington and Louisiana states are ground-based interferometers built in 2008 and in operation since 2014 (Figure 1.11). Both LIGO detectors are based on a Michelson interferometer whose perpendicular arms of the interferometer are 4km long. In these arms, Fabry-Perot cavities are used to increase the interaction time with a gravitational wave. Secondly, Virgo interferometer, located near Pisa in Italy, is also a very large Michelson interferometer with 3 km-long arms. As LIGO interferometers, Virgo is also isolated from external perturbations (mirrors and instrumentation suspended as well as the laser beams in a vacuum). The British-German GEO600 interferometer, also a Michelson interferometer has 0.6 km-long arms and collaborate regularly with LIGO Collaboration. KAGRA (Kamioka Gravitational Wave Detector) is a Japanese gravitational wave observatory which became operational at the end of 2019. It is also based on a Michelson interferometer and has a Fabry-Perot cavity of 3 km in each arm. KAGRA can be characterized as a 2.5-generation gravitational-wave telescope compared to the previous ones known as the second-generation telescopes. Indeed, KAGRA is an underground interferometer, located in the Kamioka mine, where it is protected from seismic noise and wind (Akutsu and Kagra Collaboration, 2019) and its mirrors operate at cryogenic temperature to reduce thermal noise. This interferometer began its first observing run in 2020. Finally, the Einstein Telescope, a triangular-shaped tunnel with 10 km-long arms is scheduled for construction between 2028 and 2035. This telescope will be built underground at a depth of between 250 and 300 m. The location of the telescope has not been determined yet. There are several candidates, including the border zone between Germany, the Netherlands and Belgium. This is one of the most promising sites for the Einstein Telescope, since the soft soils in this area blocks vibrations caused by human activity on the surface, enabling the underground observatory to take measurements without disturbance. In addition, good connections and a network of expertise centers and companies make this area attractive. The telescope is expected to be 1 000 times more precise than the other ones, meaning that it will be able to

observe up to 1 000 times more gravitational waves at a frequency of 100 per day (Bureau de projet Einstein Telescope, 2024).

In 2021, LIGO and Virgo interferometers were stopped over two years for maintenance work to be updated in order to improve their sensitivities. They began their fourth run (O4) of operations in May 2023. After this maintenance, they are now able to sense even fainter gravitational waves than before. The sensitivity of LIGO is approximately 160–190 Mpc while Virgo is around 60–100 Mpc during the O4. During this operational run (which is extended to 18 months) they will run in tandem with KAGRA observatory (with a sensitivity around 10 Mpc for spring 2024). The next observational run O5 is already planned to begin in 2027, after some break years to improve the mirror coatings still in development. It is crucial to understand the kilonova from various directions, from an early time, to know element abundances from observations. In these upcoming runs, multiple joint detections per year of both gravitational waves and kilonova are expected to occur (Colombo et al., 2022).



Figure 1.11: Aerian views of LIGO-Hanford (left) and LIGO-Livingston (right) (https://www.ligo.caltech.edu/page/ligo-gw-interferometer).

When considering these very sophisticated instruments, there are nevertheless limitations in the frequency range. Indeed, at low frequencies, a noise can be produced by the vibration of the ground and thus modify the recombination of the beams. Therefore, scientists have placed the best dampers on these mirrors to counteract these vibrations, in particular in LIGO and Virgo interferometers. The KAGRA observatory being located at least at 200 m below the ground surface, brings small seismic motion at low frequencies and a high stability of the detector (Akutsu and Kagra Collaboration, 2019). Then, as the mirrors are not at zero temperature, they can have vibrations due to the thermal agitation of the atoms composing them. Thus, the sensitivity is also limited in the intermediate frequencies. This is the advantage of using cryogenic mirrors as the KAGRA observatory. It allows to reduce the thermal noise as highlighted before (Akutsu and Kagra Collaboration, 2019). Finally, at high frequencies, limitations are of quantum origin and are related to the physics of the laser. The sensitivity is strongly limited in almost all frequency ranges, which explains why these instruments must be updated with the best available technology (Man, 2017).

Ultimately, the goal is to localize a source of gravitational waves anywhere in the sky. To do that, four comparable detectors need to be operating simultaneously around the earth. To increase the odds that four detectors are running at the same time, more than four detectors are needed in a network. A LIGO-India, will be built at Maharashtra in India and is expected to be operational in 2030. The construction of this observatory, similar to the LIGO described before, is a collaboration between the LIGO Laboratory and three institutes in India. When its

operational run will start, LIGO-India will significantly improve the probability that four detectors (with LIGO, Virgo and KAGRA being already operational) are operating at any given moment. This is the critical role that LIGO-India will play in the global gravitational wave detector network (LIGO-India collaboration, 2024).

1.6 GW170817 event

1.6.1 Gravitational signal

The first detection of a gravitational wave signal known as the *GW170817 event* occurred on August 17, 2017. This signal originated from the merger of two neutron stars located in the galaxy NGC 4993, which is situated at a distance of 130 million light-years. Since the orbital frequency of such a binary system is increasing while they get closer, the signal, particularly visible by LIGO-Livingston and Ligo-Hanford, draws a trace moving towards high frequencies according to time, as illustrated in Figure 1.12 (Abbott et al., 2017). The Virgo data does not show any signal, mainly because of the sensitivity constraints of the Virgo detector at that specific time. Moreover, since the source's location was in a less favorable region of the sky for this particular detector, it also contributed to the lack of signal detection (Mours et al., 2017).



Figure 1.12: Gravitational signal from the August 17, 2017 event measured by the LIGO-Hanford, LIGO-Livingston and Virgo interferometers (Abbott et al., 2017).

The signal recorded by LIGO is much longer than in the case of black hole mergers (about 100 seconds compared to a fraction of a second), showing that the two merging objects are lighter than black holes. The signal frequency indicates that these objects revolves at high speed around each other and are also very condensed. A more detailed examination of this data confirms the presence of two neutron stars, with their masses determined from the observed gravitational wave signals falling within the range of 1.17 to 1.60 times the mass of the Sun (Mours et al., 2017).

1.6.2 Electromagnetic counterpart

In Figure 1.13, a peak in the gamma-ray signal is observed (whose beginning is indicated by a green vertical line) at exactly 1.7 seconds after the detection of the gravitational waves. This peak corresponds to a short gamma-ray burst detected by the Fermi satellite and INTEGRAL (*International Gamma-Ray Astrophysics Laboratory*). This GW170817 event is very particular since it combines a gravitational wave signal and an electromagnetic wave signal (Connaughton and Goldstein, 2017; Savchenko et al., 2017). Moreover, the coincidence of both signals confirms that gravitational waves propagate at the speed of light as predicted by Albert Einstein.



Figure 1.13: Signal of the gamma-ray burst from event GW170817 detected by Fermi telescope (https://heasarc.gsfc.nasa.gov/docs/objects/heapow/archive/ transients/gw170817.html).

This signal also has surprising features. It is 100 000 times less luminous than those usually observed, which are at a greater distance than the galaxy in which this event occurred. The relativistic jet expands in a cone shape with an opening angle ranging from 5 to 10 degrees, emitted along the axis around which the two neutron stars were revolving prior to their merger. The low luminosity of the burst associated with the gravitational signal suggests that the system was observed from a sideways perspective suggesting that the primary emission had already moved past the Earth (Abbott et al., 2017).

In addition, the neutron-rich matter involved in the collision of neutron stars produces an electromagnetic counterpart in the UV, visible, and near-infrared (UVOIR). The optical and near-infrared emissions were detected at $t \approx 11$ hours (Coulter et al., 2017; Yang et al., 2017; Valenti et al., 2017), followed by the detection of a bright UV emission by Swift telescope at $t \approx 16$ hours (Evans et al., 2017). Then, X-ray and radio emissions were also detected at t = 9 days and t = 16 days, respectively (Troja et al., 2017; Hallinan et al., 2017; Mooley and Mooley, 2017) This counterpart fades rapidly and can quickly become undetectable. It is therefore important to determine as fast as possible the galaxy where these counterparts come from.

The distance of a source can be directly measured thanks to gravitational waves. For this event, the source has been estimated at 40 Mpc, that is to say 130 million light-years, with a precision

of about 10 Mpc (about 30 million light-years). However, by considering only the gravitational waves, it is not possible to determine the position of the source with precision. For this reason, it is important to consider both gravitational waves with the associated electromagnetic waves.

Moreover, the presence of Virgo, the third interferometer of the network, was essential since it brought a very high precision to localize the source as illustrated in Figure 1.14. The latter was located in a region of the sky of approximately 30 square degrees. Without the indispensable assistance provided by Virgo, the localization would have been constrained to 190 square degrees, considerably complicating the task of localizing the merger of the stars.



Figure 1.14: Sky position reconstructed for GW170817 by a fast localization algorithm using LIGO-Virgo (Abbott et al., 2017).

By considering only these 30 square degrees into the sky, the scientists had to be interested in only 50 galaxies. They quickly located the galaxy-source by visualizing a luminous point which was not present in the archival images. The so-called transient visible counterpart of the GW170817 event was detected by the SWOPE collaboration about 10 hours after the first signal alert, as shown in Figure 1.14 but also by five other international collaborations that independently performed the same detection. This counterpart, initially named SSS17a by the group from Las Campanas Observatory in Chile, was renamed AT2017gfo according to the nomenclature of the International Astronomical Union as shown in Figure 1.15 (Smartt et al., 2017).



Figure 1.15: Point source detected in the halo of the lenticular galaxy NGC 4993 (Smartt et al., 2017).

Following the visible and infrared counterpart, Chandra telescope could observe an X-ray electromagnetic signal. A few days after this detection, a counterpart in the radio range was observed by the VLA (*Very Large Array*) telescope (Nakar and Piran, 2011).

1.6.3 Analysis of the electromagnetic counterpart and production of lanthanides

Once the visible counterpart was identified, extensive observations were conducted over the subsequent hours, employing numerous ground-based and space telescopes, to enable a detailed and highly precise study of the phenomenon. This counterpart had different properties from other astrophysical phenomena observed previously. A day before the merger, the source was optically very bright (about 10^8 times brighter than the Sun at wavelengths of 0.5 μ m) but dimmed rapidly after a few days (Rosswog, 1999; Freiburghaus et al., 1999). The infrared emission (1-3 μ m) remained quite bright for almost two weeks (Rosswog et al., 2000; Goriely et al., 2011). It is, in particular, this late emission that suggests the production of lanthanides (Coté et al., 2019).

The spectrum of this counterpart is described as a blackbody spectrum suggesting that a thermal source is present (Korobkin et al., 2012; Panov et al., 2013). The succession of spectra, obtained with the X-Shooter instrument at the VLT (*Very Large Telescope*) by the GRAWITA (Pian et al., 2017) and ePESSTO (Smartt et al., 2017) collaborations, illustrated in Figure 1.16 show excellent consistency with theoretical predictions of a kilonova. Several features are important to notice in this Figure 1.16. First, the rapid cooling of the kilonova can be seen, as the light intensity decreases and the spectrum peak gradually shifts from blue to red, indicating a decrease in temperature. Moreover, after 2.5 days, the ePESSTO collaboration has detected the spectral signature of the absorption by two heavy elements, cesium and tellurium (Mours et al., 2017). More generally, the detailed modeling of the light curve and electromagnetic spectra of the kilonova reveals that the ejected material possesses significant opacity. This opacity arises from the existence of elements heavier than tellurium or cesium, such as *e.g.* lanthanides. Due to their complex atomic structure (open 4f subshell), these elements produce numerous spectral lines, as detailed in Section 1.4. Finally, the maximum of the spectrum becomes relatively weak *i.e.* the medium becomes transparent when the temperature decreases.



Figure 1.16: Spectrum of the electromagnetic emission from the August 2017 event (spectrum obtained by the GRAWITA (Pian et al., 2017) and ePESSTO (Smartt et al., 2017) collaborations).

This GW170817 signal is very interesting to study since it associates gravitational waves and electromagnetic waves. This event gave rise to a new field of astronomy known as *multi-messenger*. This illustrates the complementary nature of the gravitational data, which aids in characterizing and localizing the binary system, and the electromagnetic component, which provides insights into the events surrounding the coalescence, offering valuable additional information for locating the system.

1.7 Importance of atomic data in moderately-charged lanthanides atomic data

It is now well established that a very large part of the opacity characterizing kilonova spectrum results from the very large amount of transitions belonging to the lanthanides (Z = 57-71) (Pian et al., 2017). These elements are indeed characterized by configurations such as $4f^k$, $4f^{k-1}nl$, $4f^{k-2}nln'l'$ (k = 1-14, nl,n'l' = 5d, 6s, 6p,...) producing a large number of very close energy levels and, consequently, a multitude of spectral lines contributing in a preponderant way to the opacity. In order to study kilonova spectra it is essential to have a large amount of atomic data (such as energy levels, wavelengths and oscillator strength) as reliable as possible.

Atomic structures and radiative processes characterizing lowly-ionized lanthanides have already been the subject of various theoretical and experimental studies in recent years, such as Nd II–IV (Gaigalas et al., 2019), Nd II–III (Flörs et al., 2023), Er III (Gaigalas et al., 2020), Pr–Gd

II (Radžiūtė et al., 2020), Ce II–IV (Carvajal Gallego et al., 2021), La–Lu I–IV (Tanaka et al., 2020) and La–Yb I–IV (Fontes et al., 2020) with the aim of estimating opacities for kilonova ejecta conditions one day after the neutron star merger, *i.e.* for temperatures typically below 20 000 K (Tanaka et al., 2020). Another study about such heavy elements comes from the research group in Atomic Physics and Astrophysics of the University of Mons. Indeed, about 20 years ago, this group undertook a systematic and detailed analysis of the spectroscopic properties of the first four ionization stages of lanthanide atoms, from neutral to trebly charged. In order to allow a wide dissemination of the many new radiative parameters deduced from this work, the UMONS group has created the DREAM database (Database on Rare-Earths At Mons University) (https://hosting.umons.ac.be/html/agif/databases/dream.html) which currently contains radiative data (wavelengths, transition probabilities and oscillator strengths) on more than 72 000 spectral lines belonging to the neutral, singly-, doubly- and trebly-ionized lanthanides. These investigations gave rise to about fifty publications, the summary of which is given in a recent review paper (Quinet and Palmeri, 2020).

While the determination of these parameters has already been the subject of various studies mentioned above, the latter only concern the first degrees of ionization (up to 3+) and are therefore limited to the analysis of kilonovae in a temperature range below 20 000 K. In order to extend the modeling of this type of celestial object to higher temperatures, corresponding to the early phases of kilonovae, it is essential to know the spectroscopic properties of lanthanide ions in higher charge stages for which practically no investigation has been published to date. Indeed, the only theoretical studies concerning moderately-ionized lanthanides are the works of Banerjee et al. (2022, 2023) showed in Section 1.4 in Figure 1.9. These two publications are based on HULLAC calculations (Bar-Shalom et al., 2001) with rather limited models. In order to offer much more accurate results by improving models and by using other theoretical methods, systematic and detailed studies of the atomic structures and radiative processes characterizing these elements are therefore urgently needed. This work aims to make a significant contribution in this field as it consists of a detailed study of the radiative processes characterizing moderately-charged lanthanide ions (from 4+ to 9+) and to compute the corresponding astrophysical opacities.

As there is almost no experimental data available for these ions, our large-scale calculations are based on a multi-platform approach involving different independent theoretical approaches, such as the pseudo-relativistic Hartree-Fock (HFR) (Cowan, 1981), the fully-relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) (Grant, 2007) and Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT) (Dzuba et al., 1996) methods. In the absence of sufficient experimental data, this methodology is the only way to estimate the accuracy of the results obtained through systematic comparisons between distinct computational procedures. Theoretical approaches as well as the computational methods implementing them are detailed in the next chapter.

Chapter 2

Theoretical and computational approaches

In this chapter, we provide a comprehensive overview of the theoretical techniques employed in this study for modeling the atomic structure of lanthanides. First, a summary of the pseudo-relativistic Hartree-Fock (HFR) method, implemented in the Cowan's code (Cowan, 1981), is detailed in the first section. Then, the fully-relativistic Multi-Configurational Dirac-Hartree-Fock method (MCDHF) (Grant, 2007), implemented in the GRASP2018 computational code (Froese Fischer et al., 2019), is explained in the second section. The third method, namely the Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT) (Dzuba et al., 1996) implemented in AMBiT (Kahl and Berengut, 2019), is used to corroborate results obtained with the two other methods for some selected cases. It is important to highlight that all these methods are independent from each other which is an undeniable quality for the comparison of results.

It should be noted that all the equations written in this manuscript are formulated in Hartree atomic units, *i.e.* in the system of units where

$$m_e = 1$$
; $\hbar = 1$; $e = 1$; $4\pi\epsilon_0 = 1$,

 m_e being the electron mass, e its charge and ϵ_0 the vacuum permittivity.

2.1 Pseudo-relativistic Hartree-Fock method and corrections related to the polarization of the atomic core (HFR+CPOL)

The pseudo-relativistic HFR method consists in solving iteratively the Hartree-Fock equations by using the central field approximation. First, we remind some basic principles of the Hartree-Fock (HF) method. Then, relativistic corrections added in a perturbative way are also explained. The HFR method was improved by the Atomic Physics and Astrophysics Unit of UMONS (Quinet et al., 1999, 2002) in order to incorporate core polarization effects (HFR+CPOL). At the end of this section, we also briefly describe the procedure of the computational Cowan's code (Cowan, 1981) which implements HFR and also HFR+CPOL method.

2.1.1 Basics principle of the HF method

One way to characterize the electronic structure is to solve the Schrödinger equation, which enables the determination of eigenvalues (E_k) linked to the corresponding eigenvectors (ψ_k)

$$H\psi_k = E_k\psi_k. \tag{2.1.1}$$

The non-relativistic Hamiltonian for the atomic system studied is given by:

$$H = \sum_{i=1}^{N} \left(-\frac{1}{2}\Delta_i - \frac{Z}{r_i}\right) + \sum_{i>j} \frac{1}{r_{ij}},$$
(2.1.2)

where N is the number of electron, r_i is the distance between the i^{th} electron and the nucleus (considered here as point-like), r_{ij} is the distance between the i^{th} and the j^{th} electrons and Δ_i is the Laplacian operator acting on r_i . This problem is not solvable analytically for N > 1. Therefore, we have to use the central-field approximation in which each electron move itself independently from the other electrons in a spherically symmetric potential generated by the nucleus and the other N - 1 electrons. In this approximation, the Hamiltonian can be rewritten as:

$$H = \sum_{i=1}^{N} \left(-\frac{1}{2}\Delta_i - \frac{Z}{r_i} + V(r_i)\right),$$
(2.1.3)

where $V(r_i)$ is the spherically symmetric potential for the *i*th electron. Here, the problem becomes a one-electron problem as for the hydrogen atom, which is a problem solvable analytically. We can therefore write the wavefunction for each electron such as:

$$\phi_i(r_i, \theta_i, \Phi_i, s_i) = \frac{1}{r_i} P_{n_i l_i}(r_i) Y_{l_i}^{m_i}(\theta_i, \Phi_i) \sigma_{m_{s_i}}(s_i), \qquad (2.1.4)$$

where (r_i, θ_i, Φ_i) are the spherical coordinates, s_i the spin coordinate, $P_{nl}(r)$ is the radial part of the wavefunction, Y_l^m is a spherical harmonic and $\sigma_{m_s}(s)$ is the spin wavefunction. We can therefore build an antisymetrical atomic wavefunction by using a Slater determinant ¹:

$$\psi(q_1, ..., q_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(q_1) & \dots & \phi_1(q_N) \\ \dots & \dots & \dots \\ \phi_N(q_1) & \dots & \phi_N(q_N) \end{vmatrix},$$
(2.1.5)

where $q_i = (r_i, \theta_i, \Phi_i, s_i)$. The obtained wavefunction is an eigenfunction of the Hamiltonian. To obtain the atomic wavefunctions giving the atomic states, it is necessary to solve HF equations. The latter are obtained by applying a variational principle of minimizing the average energy E_{av} of a configuration to the radial parts. They form a system of coupled integrodifferential equations. The average energy of a configuration is defined as:

$$E_{av} = \frac{\sum_{i} (2J_i + 1)E_i}{\sum_{i} (2J_i + 1)},$$
(2.1.6)

where the sum is running over all the energy levels of the configuration. It can also be written as the sum over all the energy states of the average Hamiltonian operator H in each state $|i\rangle$:

¹A Slater determinant allows the wave function to be written as an antisymmetric product of single-electron spin-orbitals

$$E_{av} = \sum_{i \in C} \frac{\langle i|H|i\rangle}{g(C)},\tag{2.1.7}$$

where g(C) is the degeneracy of the configuration C. By developing this term, Cowan (1981) has shown that it appears electronic interaction terms that can be expressed from the Slater integrals. The generalized Slater integral R^k reflecting the electrostatic interaction between two electrons belonging to different configurations is given by:

$$R^{k}(ij;tu) = \int_{0}^{\infty} \int_{0}^{\infty} \frac{r_{min}^{k}}{r_{max}^{k+1}} P_{i}^{*}(r_{1}) P_{j}^{*}(r_{2}) P_{t}(r_{1}) P_{u}(r_{2}) \mathrm{d}r_{1} \mathrm{d}r_{2}, \qquad (2.1.8)$$

where r_{min} and r_{max} are respectively the smallest and the biggest values of r_1 and r_2 . The direct electrostatic interaction $F^k(ij) = R^k(ij;ij)$ and the exchange electrostatic interaction $G^k(ij) = R^k(ij;ji)$ which reflects interactions between two electron of the same configuration are particular cases of the generalized Slater integral. These ones exist only for some values of k: $F^k(ij)$ only exists for $k = 0, 2, 4, ..., \min(2l_i, 2l_j)$ and $G^k(ij)$ only exists for $k = |l_i - l_j|$, $|l_i - l_j| + 2, ..., l_i + l_j$. The HF equations obtained by minimizing the E_{av} for a configuration:

$$(n_1 l_1)^{w_1} (n_2 l_2)^{w_2} ... (n_q l_q)^{w_q}$$
 where $\sum_{i=1}^q w_i = N,$ (2.1.9)

are then given by:

$$\left[-\frac{d^2}{2dr^2} + \frac{l_i(l_i+1)}{2r^2} - \frac{Z}{r} + \sum_{j=1}^q (w_j - \delta_{ij}) \int_0^\infty \frac{1}{r_{max}} P_j^2(r') dr' - (w_i - 1) A_i(r) \right] P_i(r)$$

= $\epsilon_i P_i(r) + \sum_{j=1, j \neq i}^q w_j [\delta_{ij} \epsilon_{ij} + B_{ij}(r)] P_j(r),$
(2.1.10)

where

$$A_{i}(r) = \frac{2l_{i}+1}{4l_{i}+1} \sum_{k=1}^{\infty} \begin{pmatrix} l_{i} & k & l_{i} \\ 0 & 0 & 0 \end{pmatrix}^{2} \int_{0}^{\infty} \frac{2r_{min}^{k}}{r_{max}^{k+1}} P_{i}^{2}(r') \mathrm{d}r', \qquad (2.1.11)$$

$$B_{ij}(r) = \frac{1}{2} \sum_{k=1}^{\infty} \begin{pmatrix} l_i & k & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 \int_0^\infty \frac{2r_{min}^k}{r_{max}^{k+1}} P_i^2(r') P_j^2(r') \mathrm{d}r'.$$
(2.1.12)

The symbols between the parenthesis are the 3-j symbols of Wigner, w_j is the number of electrons in the subshell (n_j, l_j) and ϵ_i and ϵ_{ij} are Lagrange multiplicators introduced in the variationnal problem to impose orthonormality constraints to P_i such as:

$$\int_{0}^{\infty} P_{i}^{2}(r) \mathrm{d}r = 1 \quad \text{and} \quad \int_{0}^{\infty} P_{i}^{*}(r) P_{j}(r) \mathrm{d}r = \delta_{n_{i}, n_{j}}.$$
 (2.1.13)

Since the HF equations are coupled equations, they can only be solved by an iterative process, called the self-consistent field method. This approach involves the selection of a specific set of initial radial wavefunctions, followed by the calculation of all terms (which do not involve the one-electron radial wavefunction $P_i(r)$ for which the HF equation is solved) appearing in each HF equation with this set of radial wavefunctions. Then, the HF equations are solved one by one to obtain a new set of radial wavefunctions and the process is repeated until a certain convergence criterion on the radial wavefunctions and energies is reached.

2.1.2 Relativistic corrections (HFR method)

In order to take into account selected relativistic effects, we have to introduce mono-electronic corrections such as the mass-velocity correction, the spin-orbit correction and the Darwin term. The latter are added to the non-relativistic HF equations in a pertubative way to form the pseudo-relativistic Hartree-Fock equations (namely HFR).

Mass-velocity correction

The first adjustment introduced to the non-relativistic HF equations is the mass-velocity correction. The latter is due to the relativistic dependence of the electron's mass on its velocity. In order to obtain this correction, it is necessary to compute the difference between the relativistic energy and the non-relativistic energy of an electron, namely $E_r - E_{nr}$ where:

$$E_r = c\sqrt{c^2 + p^2} - c^2 + E_{pot},$$
(2.1.14)

and

$$E_{nr} = \frac{p^2}{2} + E_{pot}.$$
 (2.1.15)

By expanding the square root in Eq. (2.1.14) into the power series:

$$\sqrt{1 + \frac{p^2}{c^2}} \simeq 1 + \frac{1}{2}\frac{p^2}{c^2} - \frac{1}{8}\frac{p^4}{c^4},$$
(2.1.16)

which gives for the energy expression:

$$E \simeq \left(\frac{p^2}{2} + E_{pot}\right) - \frac{p^4}{8c^2} = E_{nr} - \Delta E_r.$$
(2.1.17)

For $E_{kin} \leq c^2$ higher terms can be neglected. In this approximation the last term in Eq. (2.1.17) represents the relativistic correction ΔE_r to the non-relativistic energy. The quantum mechanical value of this correction is obtained by substituting $\vec{p} \rightarrow i\hbar \vec{\nabla}$ by taking the mean value of $E_r - E_{nr}$ of a state characterized by quantum numbers (n, l, m), which leads to the expression (Demtröder, 2018):

$$\Delta E_r = \frac{\hbar^4}{8c^2} \int \psi_{n,l,m}^* \nabla \psi_{n,l,m} \mathsf{d}\tau.$$
(2.1.18)

If one takes the atomic wavefunction ψ of the hydrogen atom, we have:

$$\Delta E_r = -E_{nr} \frac{Z^2 \alpha^2}{n} \left(\frac{3}{4n} - \frac{1}{l+1/2}\right).$$
(2.1.19)

where α is the fine-structure constant which is equal to 1/137 (Demtröder, 2018).

Spin-orbit correction

The second correction is the spin-orbit correction which explains the interaction between the orbital angular momentum of an electron $(\vec{l_i})$ and its spin $(\vec{s_i})$. This interaction leads to a shift and a splitting of the energy levels. This splitting is also called the fine structure. This correction is introduced in the Hamiltonian by adding a term proportional to $\vec{l_i}.\vec{s_i}$. This factor is called the spin-orbit parameter and it is noted as ζ_{n_i,l_i} . The latter is expressed as:

$$\zeta_{n_i,l_i} = \frac{\alpha^2}{4} \int_0^\infty \frac{1}{r} \left(\frac{\mathrm{d}V}{\mathrm{d}r}\right) |P_{n_i,l_i}| \mathrm{d}r, \qquad (2.1.20)$$

where V is the central-field potential and α is the fine-structure constant.

Darwin term

The last correction is the Darwin term. This correction appears since even in a model which describes the electron as a point charge, the instantaneous position of an electron can only be defined within a volume corresponding to λ_C^3 , where λ_C represents the Compton wavelength. Its charge is therefore spread on a given volume which induce modification on its potential energy. The latter is now the weighted average of all values of the electric field within the volume λ_C^3 around r and can be written as (Demtröder, 2018):

$$\langle E_{pot}(r) \rangle = \int f(\rho) E_{pot}(r+\rho) \mathrm{d}^3 \rho,$$
 (2.1.21)

where the integral corresponds to the λ_C^3 volume around the point r. If we expand this expression in a Taylor series around the point $\rho = 0$, we obtain:

$$E_{pot}(r+\rho) = E_{pot}(r) + \left(\frac{dE_{pot}}{d\rho}\right)_{\rho \to 0}\rho + \frac{1}{2}\frac{d^2E_{pot}}{d\rho^2}\rho^2.$$
 (2.1.22)

The first term corresponds to the unperturbed energy, while the second term is zero due to the spherical symmetry of the Coulomb field (Demtröder, 2018). The third term gives the relativistic Darwin correction, which will be approximately equal to $1/c^2 \Delta E_{pot}(r)$ where Δ is the Laplacian operator. For the Coulomb potential $E_{pot} = -Z/r$, we obtain:

$$\Delta E_{pot} = 4\pi Z \delta(r). \tag{2.1.23}$$

where $\delta(r)$ is the Dirac delta function $\delta(r = 0) = 1$ for and $\delta(r \neq 0) = 0$ and the relativistic correction becomes (Demtröder, 2018):

$$\Delta E_{r,D} = 4\pi \frac{Z}{c^2} \delta(r), \qquad (2.1.24)$$

and the Darwin term is the average value of the latter (Demtröder, 2018):

$$\langle \Delta E_{r,D} \rangle = 4\pi \frac{Z}{c^2} |\psi(r=0)|^2.$$
 (2.1.25)

This term is non-zero for the s-subshell (*i.e.* l = 0), meaning that Darwin term only affects s-electrons.

2.1.3 Core-polarization corrections (HFR+CPOL method)

Within an ion, it is possible to distinguish core orbitals from valence orbitals. It is well established that the spectroscopic properties of an atom are mainly affected by the valence electrons. Therefore, the Hamiltonian can be modified by adding an approximated potential which describes the core electrons interactions. Nevertheless, it must be ensured that this simplification preserves the effects of the ionic core on the wavefunctions of valence electrons (screening effect and orthogonality of the wavefunction of a valence electron to the one of a core electron). Correlation effects can be categorized into three types: those occurring among valence

electrons, those between core electrons, and those between core and valence electrons. For heavy ions, Migdalek and Baylis (1979) developed an approach according to which the correlation between the valence electrons is represented by the configuration interaction introduced explicitly in the model while the core-valence correlation is described by a model potential reflecting the core polarization. For an ion containing N valence electrons, the one-body part of the polarization potential can be written as (Quinet et al., 1999, 2002):

$$V_{P1} = -\frac{1}{2}\alpha_d \sum_{i=1}^{N} \frac{r_i^2}{(r_i^2 + r_c^2)^3},$$
(2.1.26)

where α_d is the dipole polarizability of the core and r_c is the cut-off radius. Interactions between electric fields modified by valence electrons generate a two-particle term written as:

$$V_{P2} = -\alpha_d \sum_{i>j} \frac{\vec{r_i} \cdot \vec{r_j}}{[(r_i^2 + r_c^2)(r_j^2 + r_c^2)]^{3/2}}.$$
(2.1.27)

An additional correction was introduced by Hameed (1972). This term accounts for a more realistic core penetration of valence electrons. When introducing the core polarization into the Hamiltonian, the dipole moment operator appearing in the transition matrix must be modified. Consequently, the dipole radial integral becomes:

$$\int_{0}^{\infty} P_{nl}(r)r \left(1 - \frac{\alpha_d}{(r^2 + r_c^2)^{3/2}}\right) P_{n'l'}(r) - \frac{\alpha_d}{r_c^3} \int_{0}^{r_c} P_{nl}(r)r P_{n'l'}(r) \mathrm{d}r.$$
(2.1.28)

The α_d value can be obtained experimentally or by theoretical calculations (Fraga et al., 1976), and the r_c value, being not measurable, is taken to be the average value of the outermost orbital of the core computed by HFR.

Biémont et al. (2001) showed that HFR+CPOL calculations give similar results to a completely relativistic calculation taking into account valence interactions and core-valence interaction in an explicit way.

2.1.4 The matrix method

The matrix method also called the Slater-Condon theory is a method to solve the Schrödinger equation. We develop atomic wavefunctions Ψ^k which are eigenvectors of Hamiltonian H on a set of basis wavefunctions ψ_b in general characterized by an electronic coupling scheme as:

$$\Psi^k = \sum_b x_b^k \psi_b. \tag{2.1.29}$$

The basis functions are assumed to take part of a set of orthonormal function such as:

$$\langle \psi_b | \psi_{b'} \rangle = \delta_{bb'}. \tag{2.1.30}$$

The series corresponding to Ψ^k is in general an infinite serie (in other words, the basis is made up of an infinite number of basis states). However, in practice, it is truncated by choosing electronic configurations which will be then introduced explicitly into the model. It is thus necessary that these basis functions be of an appropriate type to be included in Eq. (2.1.29). If one consider a set of M suitable basis functions and want to determine the values of the M
expansion coefficients x_b , by substituting Eq. (2.1.29) in the Schrödinger equation Eq. (2.1.1), we have:

$$\sum_{b=1}^{M} H x_b^k \psi_b = E^k \sum_{b=1}^{M} x_b^k \psi_b.$$
 (2.1.31)

If we multiply this equation from the left by ψ_b (a basis function), integrate over all 3N space coordinates and sum over both possible directions of each of the N spins, we have:

$$\sum_{b=1}^{M} H_{bb'} x_b^k = E^k \sum_{b=1}^{M} x_b^k \text{ where } H_{bb'} = \langle \psi_b | H | \psi_b' \rangle.$$
 (2.1.32)

The $H_{bb'}$ is the matrix element of the Hamiltonian operator between the basis functions b and b'. The latter equation has a set of M simultaneous linear homogeneous equations in the M unknowns $x_{b'}^k$. This set of equations has a non-trivial solution if the determinant of the matrix $(H_{bb'} - E^k \delta_{bb'})$ is zero. To do that, it is possible to expand this determinant into a polynomial of degree M in E^k . Each value of E^k substituted in Eq. (2.1.32) gives M - 1 independent equations for the M - 1 ratios x_b^k/x_i^k with $b \neq i$. To have a normalized Ψ^k , the value of x_i^k has to be chosen such that:

$$\sum_{b} (x_b^k)^2 = 1. \tag{2.1.33}$$

For larger M, the only practical procedure is to numerically diagonalize the Hamiltonian matrix H, if one writes the set of expansion coefficients in the form of:

$$X^{k} = \begin{pmatrix} x_{1}^{k} \\ x_{2}^{k} \\ x_{3}^{k} \\ \vdots \\ \vdots \\ \vdots \end{pmatrix}, \qquad (2.1.34)$$

Eq. (2.1.32) can be written as the single matrix equation such as:

$$\begin{pmatrix} H_{11} & \dots & H_{1n} \\ \dots & \dots & \dots \\ H_{n1} & \dots & H_{nn} \end{pmatrix} \begin{pmatrix} x_1^k \\ \dots \\ x_n^k \end{pmatrix} = E^k \begin{pmatrix} x_1^k \\ \dots \\ x_n^k \end{pmatrix}.$$
 (2.1.35)

The diagonalization of the Hamiltonian will thus provide the eigenvalues and the mixing coefficients x_b^k . The latter, *via* the series development, will finally give the expression of the atomic wavefunctions Ψ^k .

2.1.5 Line strengths, transition probabilities and oscillator strengths

The so-called configuration interaction (*i.e.* interactions between the basis states belonging to different configurations when atomic wavefunctions do not belong to a pure state but rather to a superposition of states) reflected by Eq. (2.1.29) is characterized by a truncated summation. The latter introduces undesired effects in the calculation of transition probabilities because of the inaccuracies that arise during the truncation process, known as cancellation effects.

The latter can result in a transition being calculated with a much lower intensity than its real value. To evaluate the importance of these cancellation effects for a calculated transition (between a $|\Psi_i\rangle$ state and a $|\Psi_j\rangle$ state), the cancellation factor (CF) is employed. It can be derived from the line strength of the transition defined as:

$$\sqrt{S_{ij}} = \langle \Psi_i | P^{(1)} | \Psi_j \rangle. \tag{2.1.36}$$

The line strength (for an E1 transition) is the square of the electric dipole transition matrix element $P^{(1)}$ between the states considered: $S_{ij} = |\langle \Psi_i | P^{(1)} | \Psi_j \rangle|^2$. If one expands Ψ_i (and Ψ_j) in a suitable set of basis functions ψ_c (or ψ_b), one gets:

$$\sqrt{S_{ij}} = \sum_{b} \sum_{c} x_j^b x_i^c \langle \psi_c | P^{(1)} | \psi_b \rangle.$$
(2.1.37)

The CF factor is then defined as:

$$CF_{ij} := \left(\frac{\sum_{b} \sum_{c} x_{j}^{b} x_{i}^{c} \langle \psi_{c} | P^{(1)} | \psi_{b} \rangle}{\sum_{b} \sum_{c} |x_{j}^{b} x_{i}^{c} \langle \psi_{c} | P^{(1)} | \psi_{b} \rangle|}\right)^{2}.$$
(2.1.38)

For a given transition, the smaller is the CF-value, the less reliable the corresponding values are (namely transition probability and oscillator strength). In this work, we will consider that the values of radiative parameters calculated with CF < 0.05 are unreliable and should be treated with caution.

The transition probabilities and oscillator strengths can be defined using the expression of line strengths written in Eq. (2.1.37). The weighted transition probability from a state $\gamma' J' M'$ to all states M of the level γJ can be calculated such as:

$$gA = (2J+1)A = 2.0261 \times 10^{-6} \sigma^3 S, \qquad (2.1.39)$$

where σ is the wavenumber (cm⁻¹). Another important quantity is the oscillator strength, which is also related to the line strength S. For absorption, it can be written as:

$$f_{ij} = \frac{(E_j - E_i)}{3(2J+1)}S,$$
(2.1.40)

where $E_j - E_i$ is the transition energy and refers to the total probability of absorption from a specific state of the lower level *i* to all (2J'+1) states of the upper level *j*. Concerning emission processes, the oscillator strength can be written as:

$$f_{ji} = \frac{(E_i - E_j)}{3(2J' + 1)}S.$$
(2.1.41)

A weighted oscillator strength can be also defined just as for the weighted transition probability such as:

$$gf = (2J+1)f_{ij} = -(2J'+1)f_{ji} = 3.0376 \times 10^{-6}\sigma S.$$
(2.1.42)

It is also possible to link both quantities, weighted transition probability and weighted oscillator strength such as:

$$gA = 0.66702 \ \sigma^2 gf. \tag{2.1.43}$$

It is also important to highlight that the g (*i.e.* (2J+1)) appearing to weight the transition probability and the oscillator strength in emission refers to the upper level while for the oscillator strength in absorption g refers to the lower level.

2.1.6 Cowan's code procedure

The Cowan's code, which implements the HFR method, enables the modeling of the atomic structure for a given atom. This approach computes the radial and angular parts of the wavefunction, enabling the determination of energy levels and the atomic system's wavefunctions. This is achieved through the diagonalization of the Hamiltonian H using the Slater-Condon method, as detailed in the previous subsections.

The procedure to calculate atomic parameters includes four different programs used in a row. All these programs are executed *ab initio*, meaning that parameters can be calculated without introducing any experimental data. The first program RCN requires the introduction of configurations considered within the *in36* file. This program calculates radial parts $(P_{nl}(r))$ of monoelectronic wavefunctions by solving HF equations with the self-consistent field approximation. It also calculates the monoconfigurational parameters of each configuration, the average energy (E_{av}) , electrostatic Slater interaction such as $F^k(ij)$ and $G^k(ij)$ and also the spin-orbit parameter ζ_{nl} .

The second program, RCN2, then calculates the Slater integrals R^k , which reflect the electostatic interaction between different electronic configurations and the radial parts of the transition amplitudes such as the electric dipole transition radial integrals. It also includes scaling factors (SF) in the *in2* file. In fact, as we cannot model the entire configuration interactions (because we choose to enter a finite and limited number of configurations) it creates a systematic error which consist to have values of the radial Slater integrals F^k , G^k and R^k calculated too high compared to their optimal values. Therefore, we introduce these scaling factors (SF) to have a better agreement between the calculated energy levels and experimental values. For moderatelycharged heavy elements such as considered in this thesis, F^k , G^k and R^k were arbitrarily scaled down by a factor 0.90 while the spin-orbit parameters (ζ_{nl}), computed using the Blume-Watson method, were kept at their *ab initio* values, as recommended by Cowan (1981).

The final program, namely RCG, builds the Hamiltonian using various parameters calculated by the RCN and RCN2 programs (F^k , G^k , R^k , ζ_{nl} and E_{av}). By diagonalizing the Hamiltonian, we have then access to eigenvalues, mixing coefficients and eigenvectors of the atomic system. Then, electric dipole transitions (E1) are calculated in order to obtain radiative parameters such as transition probabilities, oscillator strengths, wavelengths and cancellation factors.

As mentioned previously, all these programs can be run in a row. For all of the ions considered in this work, we used the HFR method without using the polarization corrections since we demonstrated in Deprince et al. (2023) that these corrections have a relatively weak impact on opacities for heavy elements. Here is a summary of the main steps when using Cowan's code.

RCN	Monoelectronic wavefunctions radial parts calculation
\downarrow	
RCN2	Slater interaction parameters R^k calculation + introduction of scaling factors
\downarrow	
RCG	Diagonalization of the Hamiltonian \Rightarrow Generation of atomic data

2.2 Multi-Configurational Dirac-Hartree-Fock method (MCDHF)

The MCDHF approach (Grant, 2007) consists in solving approximately the Dirac equation for each bound electron of the considered atom by using the central-field approximation. Firstly, some fundamental notions of relativistic quantum mechanics are reminded in the beginning of this section. Then, theoretical principles of MCDHF method are explained such as the construction of the Hamiltonian. After the description of the method to obtain spin-orbitals, the corrective terms related to quantum electrodynamics (QED) and the transition probabilities are also detailed. Finally, we briefly describe the procedure of the computational program GRASP2018, (Froese Fischer et al., 2019), used to calculate the atomic structures elements.

2.2.1 Relativistic quantum mechanics: the hydrogen atom problem

In relativistic quantum mechanics, the motion of a free electron is described by the Dirac equation

$$(i\gamma^{\mu}\partial_{\mu} - c)\psi = 0, \qquad (2.2.1)$$

where γ^{μ} represent the (4×4) Dirac matrices with $\mu = 0, 1, 2, 3$ and are written as:

$$\gamma^{0} := \begin{pmatrix} \mathbb{1} & 0\\ 0 & -\mathbb{1} \end{pmatrix}; \quad \gamma^{i} := \begin{pmatrix} 0 & \sigma^{i}\\ -\sigma^{i} & 0 \end{pmatrix}, \qquad (2.2.2)$$

where i = 1,2,3, σ^i are the (2×2) Pauli matrices, c is the speed of the light in the vacuum, ψ is the four components Dirac spinor solution of the equation and ∂_{μ} is the partial derivative acting on the Dirac spinor.

When we consider the hydrogen atom (monoelectronic case), *i.e.* one electron in a Coulomb potential := $V_{\text{nucl}}(r)$ (*i.e.* spherically symmetric potential generated by the nucleus), it is interesting to determine the bound states of this electron to know the energy levels. To do that, we have to find the eigenvectors ψ of the monoelectronic Dirac Hamiltonian operator h_D :

$$h_D \psi = E \psi, \qquad (2.2.3)$$

where
$$h_D = c\vec{\alpha}.\vec{p} + (\beta - 1)c^2 + V_{\text{nucl}}(r)$$
,

where operators α^i with i = 1,2,3 and β are defined from the Dirac matrices Eq. (2.2.2) such as

$$\alpha^i := \gamma^0 \gamma^i \; ; \quad \beta := \gamma^0. \tag{2.2.4}$$

If we treat the nucleus as point-like, then the nuclear potential included in the monoelectronic Hamiltonian in Eq. (2.2.3) can be written as: $V_{\text{nucl}}(r) = -Z/r$.

The eigenvectors of the Hamiltonian written in Eq. (2.2.3) can be noted in spherical coordinates as

$$\psi(r,\theta,\phi) = \frac{1}{r} \begin{pmatrix} P_{n,\kappa}(r) & \chi_{\kappa,m}(\theta,\phi) \\ iQ_{n,\kappa}(r) & \chi_{-\kappa,m}(\theta,\phi) \end{pmatrix}, \qquad (2.2.5)$$

where $P_{n,\kappa}(r)$ and $Q_{n,\kappa}(r)$ are respectively the large and the small radial components which are solutions of a system of differential equations (analytically solvable) and $\chi_{\kappa,m}(\theta,\phi)$ are the angular parts, which are eigenvectors of \vec{j}^2 , j_3 , \vec{l}^2 and \vec{s}^2 (where \vec{j} , \vec{l} , \vec{s} are respectively the total angular moment, the orbital angular moment and the spin, with $\vec{j} = \vec{l} + \vec{s}$). The $\chi_{\kappa,m}(\theta, \phi)$ are also eigenvectors of the operator

$$K = -(1 + \vec{\sigma}.\vec{l}), \qquad (2.2.6)$$

with eigenvalues

$$\kappa = \left(j + \frac{1}{2}\right)\eta \quad \text{when} \quad l = j + \frac{1}{2}\eta \quad \text{with} \quad \eta = \pm 1, \tag{2.2.7}$$

which makes it possible to clarify the angular parts such as (Grant, 2007)

$$\chi_{\kappa,m}(\theta,\phi) = \sum_{\sigma=\pm\frac{1}{2}} (l,m-\sigma,1/2,\sigma|l,1/2,j,m) Y_l^{m-\sigma}(\theta,\phi)\psi_{\sigma},$$
(2.2.8)

with ψ_{σ} basis spinors with two components:

$$\psi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} et \quad \psi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

2.2.2 Basic principle of the MCDHF method

Polyelectronic case and atomic state functions

When we consider an atom with N electrons, the corresponding relativistic Hamiltonian is given by the Dirac-Coulomb Hamiltonian

$$H_{DC} = \sum_{i=1}^{N} h_D(\vec{r_i}) + \sum_{i>j} \frac{1}{r_{ij}},$$
(2.2.9)

where $r_{ij} = |\vec{r_i} - \vec{r_j}|$ and $h_D(\vec{r_i})$ is the monoelectronic Dirac Hamiltonian in Eq. (2.2.3) for the *i*th considered electron. Considering the central-field approximation, each electron is assumed to move in a spherically symmetric potential created by the nucleus and the other N - 1 electrons of the atom, noted as U(r). This allows us to modify the single-electron Hamiltonian operator in Eq. (2.2.3) as

$$\tilde{h}_D = c\vec{\alpha}.\vec{p} + (\beta - 1)c^2 + V(r), \qquad (2.2.10)$$

where V(r) = -Z/r + U(r). Therefore, we can rewrite the Dirac-Coulomb Hamiltonian as

$$\tilde{H}_{DC} = \sum_{i=1}^{N} \tilde{h}_D(\vec{r_i}).$$
(2.2.11)

By considering this approximation, it is thus possible to write the eigenstates of the Hamiltonian in the same way as for the hydrogen atom, *i.e.* Eq. (2.2.5). The difference with the former is the determination of the radial parts $P_{n,\kappa}(r)$ and $Q_{n,\kappa}(r)$ through the self-consistent field method by solving a system of coupled differential equations.

An atomic state function (ASF) describing a stationary atomic state of parity π characterized by the total angular momentum quantum number J, of projection M is represented by $\Psi(\pi, J, M)$. A configuration state function (CSF) is represented by $\Phi(\gamma, \pi, J, M)$, where γ contains all the information necessary to uniquely define the CSF (the coupling scheme and the orbital occupancy numbers). These CSFs are constructed from Slater determinants (as mentioned previously, it enables the wavefunction to be expressed as an anti-symmetric combination of individual single-electron spin-orbitals). When the MCDHF method is used, the basic step is to expand each $\Psi(\pi, J, M)$ ASF into a linear combination of $\Phi(\gamma, \pi, J, M)$ CSFs as follows:

$$\Psi(\pi, J, M) = \sum_{r=1}^{n_c} c_r \Phi(\gamma_r, \pi, J, M), \qquad (2.2.12)$$

where c_r are the mixing coefficients and n_c is the number of CSFs in the chosen model. The coefficients must satisfy the normalization condition such that

$$\sum_{r=1}^{n_c} |c_r|^2 = 1.$$
(2.2.13)

When orbitals are optimized, these mixing coefficients can be determined using the configuration interaction method. The energy of an atom in a Γ state described by an ASF with a form such that the expression Eq. (2.2.12) is written:

$$E_{\Gamma} = \vec{c_{\Gamma}}^{\dagger} H \vec{c_{\Gamma}}, \qquad (2.2.14)$$

where H is the Hamiltonian matrix in the chosen basis of the CSFs and $\vec{c_{\Gamma}}$ is a column vector whose components are the mixing coefficients of the ASF which describes the atomic state Γ with the normalization condition Eq. (2.2.13), which is rewritten such as $\vec{c_{\Gamma}}^{\dagger}\vec{c_{\Gamma}} = 1$. Finding the eigenstates of the Hamiltonian thus involves to solve the following equation:

$$\tilde{H}_{DC}\vec{c_{\Gamma}} = E_{\Gamma}\vec{c_{\Gamma}}.$$
(2.2.15)

Eigenvalues and eigenvectors are obtained by diagonalizing the Hamiltonian. These correspond to the atomic energy levels and mixing coefficients of the considered ASF and allow us to describe the atomic state.

Construction of the Hamiltonian matrix in the selected CSF basis

In order to solve Eq. (2.2.15), the Hamiltonian must be constructed. The elements of the Hamiltonian matrix can be expressed from the angular coefficients which depend only on the angular parts of the chosen CSFs and from monoelectronic and bi-electronic radial integrals (Grant, 2007).

The monoelectronic radial integral for an electron initially in an orbital a (this orbital being characterized by the quantum numbers n_a , κ_a) is written as:

$$I(ab) = \delta_{\kappa_a \kappa_b} \int_0^\infty \left[cQ_a^*(r) \left(\frac{d}{dr} + \frac{\kappa_b}{r} \right) P_b(r) - cP_a^*(r) \left(\frac{d}{dr} - \frac{\kappa_b}{r} \right) Q_b(r) - 2c^2 Q_a^*(r) Q_b(r) + V_{\text{nucl}}(r) [P_a^*(r) P_b(r) + Q_a^*(r) Q_b(r)] \right] dr.$$
(2.2.16)

The bi-electronic radial integral describing the electrostatic interaction between two electrons that may belong to two different configurations is given as a generalized relativistic Slater integral and is denoted $R^k(abcd)$:

$$R^{k}(abcd) = \int_{0}^{\infty} \left[\left(P_{a}^{*}(r)P_{c}(r) + Q_{a}^{*}(r)Q_{c}(r) \right) \frac{1}{r} Y^{k}(bd;r) \right] \mathrm{d}r, \qquad (2.2.17)$$

where Y is the relativistic Hartree function and is defined as

$$Y^{k}(bd;r) = r \int_{0}^{\infty} U^{k}(r,s) \Big(P_{b}^{*}(s)P_{d}(s) + Q_{b}^{*}(s)Q_{d}(s) \Big) \mathrm{d}s, \qquad (2.2.18)$$

with

$$U^{k}(r,s) = \begin{cases} \frac{r^{k}}{s^{k+1}} & \text{if } r \leq s \\ \frac{s^{k}}{r^{k+1}} & \text{if } r > s. \end{cases}$$
(2.2.19)

The direct and exchange radial integrals, $F^k(ab)$ and $G^k(ab)$ respectively, are two special cases of the Slater integral in a monoconfiguration case. The direct radial integral reflects the direct electrostatic interaction, while the second describes the electrostatic exchange interaction between two electrons of the same configuration. They are written as:

$$F^{k}(ab) = R^{k}(abab)$$
; $G^{k}(ab) = R^{k}(abba).$ (2.2.20)

The diagonal elements of the Hamiltonian matrix in the chosen CSF basis are written as

$$H_{rr} = \sum_{a=1}^{n_o} \left(q_r(a) I(aa) + \sum_{b \ge a}^{n_o} \left[\sum_{k=0,2,\dots}^{k_o} f_r^k(ab) F^k(ab) + \sum_{k=k_1,k_1+2,\dots}^{k_2} g_r^k(ab) G^k(ab) \right] \right),$$
(2.2.21)

where n_o is the number of orbitals, $q_r(a)$ is the number of occupancy of an orbital a, *i.e.* the number of electrons in that orbital represented by the quantum numbers (n_a, κ_a) and $f_r^k(ab)$ $g_r^k(ab)$ are angular coefficients whose general expressions are defined by Grant (2007). They depend on the coupling scheme between equivalent (those on the same subshell) and non-equivalent electrons (those on different subshells). Therefore, they also depend on the number of occupancy of each subshell. The coupling scheme used in the MCDHF method in order to construct the CSFs is a jj coupling. In this coupling scheme, the electrons of the same subshell a, with occupation number $q(a) \leq 2j_a + 1$, are coupled together in jj coupling to give an angular momentum J_a to each subshell. Then, successive subshell a and b of angular momentum J_a and J_b are coupled in a jj manner to give an intermediate angular momentum X_1 which is coupled with the angular momentum J_c of the following subshells are coupled to give a total angular momentum J. It can be summarized as follows:

$$(...((J_a J_b) X_1 J_c) X_2 ...) J.$$
(2.2.22)

In Eq. (2.2.21), the limits of summation k_0 , k_1 and k_2 are given by:

$$k_{0} = (2j_{a} - 1)\delta_{ab},$$

$$k_{1} = \begin{cases} |j_{a} - j_{b}| & \text{if } \kappa_{a}\kappa_{b} > 0 \\ |j_{a} - j_{b}| + 1 & \text{if } \kappa_{a}\kappa_{b} < 0, \end{cases}$$

$$k_{2} = \begin{cases} j_{a} + j_{b} & \text{if } j_{a} + j_{b} + k \text{ is even} \\ j_{a} + j_{b} - 1 & \text{otherwise.} \end{cases}$$
(2.2.23)

The non-diagonal elements $(r \neq s)$ of the Hamiltonian matrix in the considered CSF basis, which reflect the configuration interactions between the different CSFs, are expressed as:

$$H_{rs} = \sum_{a,b} t_{rs}(ab)I(ab)\delta_{\kappa_a\kappa_b} + \sum_k \sum_{a,b,c,d} v_{rs}^k(abcd)R^k(abcd), \qquad (2.2.24)$$

where $t_{rs}(ab)$ and $v_{rs}^k(abcd)$ are angular coupling coefficients of the same form as those appearing in Eq. (2.2.21) and whose expressions are given by Grant (2007). They also depend on the coupling scheme and the subshells a,b,c and d contributing to H_{rs} .

Obtaining spin-orbitals by the MCDHF equations

It remains to optimize the radial parts in order to obtain the spin-orbitals. To do this, a system of integro-differential equations must be solved. Such a system of equations is obtained by applying a variational principle to an energy functional of atomic states. This energy functional has to be stationary with respect to the variations of the radial parts of the spin-orbitals.

Let the energy functional be such that:

$$\varepsilon = \sum_{r=1}^{n_c} \sum_{s=1}^{n_c} d_{rs} H_{rs} + \sum_a \sum_b (1 - \delta_{ab}) \bar{q}(a) \epsilon_{ab}(a|b), \qquad (2.2.25)$$

where ϵ_{ab} are the Lagrange multipliers ensuring the orthonormality of the radial parts of the spin-orbitals, $\bar{q}(a)$ is the generalized occupation number and is defined as:

$$\bar{q}(a) := \sum_{r=1}^{n_c} d_{rr} q_r(a),$$
(2.2.26)

and where

$$(a|b) = \int_0^\infty \left(P_a^*(r) P_b(r) + Q_a^*(r) Q_b(r) \right) \mathrm{d}r.$$
 (2.2.27)

The d_{rs} coefficients noted in Eq. (2.2.25) are generalized statistical weights which may be expressed differently depending on the mode used:

1. If one uses the OL (Optimal Level) mode, the optimization is done on one ASF at a time, each ASF will be optimized independently from the others. Spin-orbitals obtained can thus vary from one ASF to another. For a certain atomic state i, the weights d_{rs} are such that:

$$d_{rs} = c_{ri}c_{si}.\tag{2.2.28}$$

2. The EOL (Extended Optimal Level) mode allows the optimization to be performed on a set of levels. The generalized weights are given by:

$$d_{rs} = \frac{1}{n_L} \sum_{i=1}^{n_L} c_{ri} c_{si}, \qquad (2.2.29)$$

where n_L is the number of chosen levels (with $n_L < n_c$). In this case, the same set of spin-orbitals is used to describe the set of ASFs corresponding to the chosen energy levels when constructing the energy functional ε .

3. The AL (Average Level) mode optimizes the trace of the Hamiltonian matrix. Different from the OL and EOL modes, this mode optimizes all energy levels in a global way. The generalized weights are independent of the mixing coefficients and each CSF is weighted by its own statistical weight:

$$d_{rs} = \delta_{rs} \frac{2J_r + 1}{\sum_{t=1}^{n_c} (2J_t + 1)}.$$
(2.2.30)

4. The EAL (Extended Average Level) mode allows the optimization of a weighted trace of the Hamiltonian matrix. The weights, being independent of the mixing coefficients, can therefore be chosen by the user.

By applying the variational principle to the energy functional of a relativistic orbital *a*, we derive a set of coupled integro-differential equations, known as MCDHF equations, characterized as follows:

$$\begin{cases} -\frac{Z - Y(a;r)}{r} P_a(r) + c\left(-\frac{d}{dr} + \frac{\kappa_a}{r}\right) Q_a(r) - \epsilon_{aa} P_a(r) = -X_{+1}(a;r) \\ c\left(\frac{d}{dr} + \frac{\kappa_a}{r}\right) P_a(r) + \left(-2c^2 - \frac{Z - Y(a;r)}{r}\right) Q_a(r) - \epsilon_{aa} Q_a(r) = -X_{-1}(a;r), \end{cases}$$
(2.2.31)

with the normalization condition

$$\int_0^\infty (P_a^*(r)P_a(r) + Q_a^*(r)Q_a(r))\mathrm{d}r = 1, \qquad (2.2.32)$$

where Y(a; r) is the direct interaction potential and X_{α} with $\alpha = \pm 1$ is the exchange interaction potential. The expression for the direct interaction potential is given by:

$$Y(a;r) = \sum_{k} \sum_{b=1}^{n_0} \left[y^k(ab) Y^k(bb;r) - \sum_{c=1}^{n_0} y^k(abac) Y^k(bc;r) \right],$$
 (2.2.33)

with Y^k being the relativistic Hartree function given in Eq. (2.2.18) and $y^k(ab)$ is described such that:

$$y^{k}(ab) = \frac{1+\delta_{ab}}{\bar{q}(a)} \sum_{r=1}^{n_{c}} d_{rr} f_{r}^{k}(ab), \qquad (2.2.34)$$

$$y^{k}(abac) = \frac{1}{\bar{q}(a)} \sum_{r=1}^{n_{c}} \sum_{s=1}^{n_{c}} d_{rs} v_{rs}^{k}(abac).$$
(2.2.35)

The expression for the exchange interaction potential is given by:

$$X_{\beta}(a,r) = -\sum_{b \neq a} \delta_{\kappa_{a}\kappa_{b}} \epsilon_{ab} R_{\gamma_{b}\beta_{\kappa_{b}}}(r) + \sum_{k} \left[\sum_{b \neq a} x^{k}(ab) \frac{Y^{k}(ba;r)}{r} R_{\gamma_{b}\beta_{\kappa_{b}}}(r) - \sum_{bcd} \left(1 - \delta_{ac} x^{k}(abcd) \frac{Y^{k}(bd;r)}{r} R_{\gamma_{c}\beta_{\kappa_{c}}}(r) \right) \right],$$

$$(2.2.36)$$

with

$$R_{\gamma,\beta_{\kappa}}(r) = \begin{cases} P_{\gamma,\kappa}(r) & \text{if } \beta = +1\\ Q_{\gamma,\kappa}(r) & \text{if } \beta = -1, \end{cases}$$
(2.2.37)

and where

$$x^{k}(ab) = \frac{1}{\bar{q}(a)} \sum_{r=1}^{n_{c}} d_{rr} g_{r}^{k}(ab), \qquad (2.2.38)$$

$$x^{k}(abcd) = \frac{1}{\bar{q}(a)} \sum_{r=1}^{n_{c}} \sum_{s=1}^{n_{c}} d_{rs} v^{k}_{rs}(abcd).$$
(2.2.39)

The only way to solve this system is by an iterative method. The technique used is the selfconsistent field (SCF) which is applied to obtain the radial parts P(r) and Q(r) of each spinorbital written in Eq. (2.2.5). The SCF method is divided into three parts:

- (i) Choice of initial radial functions P(r) and Q(r) (for example the radial parts of the screened hydrogenic spin-orbitals),
- (ii) Calculation of all terms appearing in the MCDHF equations with the radial parts chosen in (i),
- (iii) Solving the MCDHF equations to obtain new radial functions.

These steps are repeated iteratively until a certain convergence criterion is reached.

2.2.3 Quantum electrodynamics corrections

In a relativistic context, the Coulomb interaction term is not sufficient to describe the interactions between the bound electrons of atoms. Indeed, it is necessary to consider some corrections from quantum electrodynamics (QED). In this context, the most important corrections are the Breit transverse interaction, self-energy and vacuum polarization. They are added in a perturbative way to the Hamiltonian to solve the eigenvalue equation in order to correct ASFs as well as the energy levels. Each of these QED contributions is briefly described below.

Breit transverse interaction.

The electron-electron scattering is explained by the exchange of a virtual photon. The Feynman diagram representing this interaction is shown in Figure 2.1.



Figure 2.1: Feynman diagram representing the electron-electron scattering (transverse interaction).

The transverse interaction is the first-order correction to the Coulomb interaction term between two bound electrons (one belonging to an i orbital and the other to a j orbital) in an atom resulting from the exchange of a virtual photon between them. This correction is described by

a transverse interaction Hamiltonian operator added to the Dirac-Coulomb Hamiltonian mentioned above. This operator is written as follows (Grant, 2007)

$$B_{ij}^{T} = -\vec{\alpha_{i}}.\vec{\alpha_{j}}\frac{e^{i\omega_{ij}r_{ij}/c}}{r_{ij}} - (\vec{\alpha_{i}}.\vec{\nabla_{ij}})(\vec{\alpha_{j}}.\vec{\nabla_{ij}})\frac{e^{i\omega_{ij}r_{ij}/c} - 1}{\omega_{ij}^{2}r_{ij}/c^{2}},$$
(2.2.40)

where $\vec{\alpha_i} = (\alpha_i^1, \alpha_i^2, \alpha_i^3)$ is a vector whose components are the three Dirac matrices cited in Eq. (2.2.4) acting on an electron that occupies the *i* orbital, $r_{ij} = |\vec{r_i} - \vec{r_j}|$ and ω_{ij} is the frequency of the virtual photon exchanged.

Self-energy

The self-energy correction is a second-order correction corresponding to the phenomenon whereby the electron spontaneously emits a virtual photon of energy ΔE and reabsorbs it after a certain time Δt such that the Heinsenberg uncertainty principle $\Delta E.\Delta t \geq \hbar$ is satisfied. Such a phenomenon is described by the Feynman diagram in Figure 2.2. It contributes to the mass-energy of electrons through the interaction of the electron with its own electromagnetic field, which results in the modification of the electronic structure of atoms.



Figure 2.2: Feynman diagram representing the self-energy.

Vacuum polarization

The polarization of the vacuum is another second-order correction of the QED theory. The latter states that an energy fluctuation ΔE of the vacuum can allow the creation of an electron-positron pair annihilating after a certain time Δt such that $\Delta E.\Delta t \ge \hbar$ is satisfied. The Feynman diagram describing this phenomenon is shown in Figure 2.3. Dipoles appear spontaneously from the vacuum for very short periods of time, thus modifying the surrounding electromagnetic field. Indeed, an electron interacting with these dipoles disturbs the spatial distribution of the latter, giving rise to a *polarization of the vacuum* as well as a modification of the electromagnetic field generated by the electron (spreading of its charge). The electronic structure of the atoms is therefore also modified.



Figure 2.3: Feynman diagram representing the vacuum polarization.

2.2.4 Transition probabilities

When the electronic structure of an atom is defined, it is possible to calculate the radiative transitions occurring within that atom and their corresponding transition probabilities. The latter are defined as the rate of spontaneous emission of a photon per unit of time for each of

the possible radiative de-excitation paths of the atom. These probabilities are obtained from the calculation of relativistic line strengths (*i.e.* matrix elements of an electromagnetic transition operator described as a multipole expansion) between ASFs corresponding to two atomic states involved in each transition. It is also convenient to define the absorption oscillator strength as

$$f_{ab} = -\frac{c}{2\omega^2} \frac{2j_b + 1}{2j_a + 1} A_{ab},$$
(2.2.41)

where ω is the angular frequency associated with the transition, c is the speed of light and A_{ab} is the relativistic transition probability for a transition from a b level to an a level (where the b level has a higher energy than the a level), which is written as follows (Grant, 2007):

$$A_{ab} = 2\alpha\omega \frac{2j_a + 1}{2K + 1} \begin{pmatrix} j_b & K & j_a \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}^2 |M_{ab}|^2, \qquad (2.2.42)$$

where α is the fine-structure constant, ω is the angular frequency associated with the transition, K is the order of the electric or magnetic multipole transition, the symbol in brackets is a 3-j Wigner symbol, which is written using Clebsh-Gordan coefficients such that:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-1)^{j_1 - j_2 - m_3}}{\sqrt{2j_3 + 1}} (j_1 m_1 j_2 m_2 | j_3 (-m_3)),$$
(2.2.43)

and M_{ab} is a function of ω depending on the electrical or magnetic character of the transition as well as the chosen gauge.

In atomic physics, it is generally common to work with a gauge other than the Lorentz gauge for the potential quadrivector. It is common to use either the Babushkin gauge or the Coulomb gauge. In the framework of non-relativistic quantum mechanics, the transition operator between an initial and a final state is either expressed in the position representation (*i.e.* length gauge) or in the momentum representation (*i.e.* velocity gauge). The relativistic transition operator computed in the Babushkin gauge relates, in the non-relativistic limit, to the transition operator computed in the length gauge, whereas the relativistic transition operator computed in the Coulomb gauge relates to the transition operator computed in the velocity gauge.

The computation of transition probabilities is carried out in either of these two gauges (Babushkin and Coulomb) in order to compare the results obtained. To verify the reliability of the latter, the gauge invariance of the theory of electromagnetism guarantees that the same theoretical results must be obtained in both gauges. In the case of electric multipole transitions, M_{ab} depends linearly on a parameter G which is the gauge parameter. In the Coulomb gauge, it is zero while in the Babushkin gauge, it is $[(K + 1)/K]^{1/2}$. Therefore, M_{ab} is written:

$$M_{ab}(\omega, G) = M_{ab}(\omega, 0) + GM_{ab}(\omega), \qquad (2.2.44)$$

where

$$M_{ab}(\omega,0) = -i^{k} \left[\left(\frac{K}{K+1} \right)^{1/2} \left[(\kappa_{a} - \kappa_{b}) I_{K+1}^{+} + (K+1) I_{K+1}^{-} \right] - \left(\frac{K+1}{K} \right)^{1/2} \left[(\kappa_{a} - \kappa_{b}) I_{K-1}^{+} + K I_{K-1}^{-} \right] \right],$$
(2.2.45)

and

$$\tilde{M}_{ab}(\omega) = -i^{k} \Big[(\kappa_{a} - \kappa_{b}) I_{K+1}^{+} + (K+1) I_{K+1}^{-} \\ + (\kappa_{a} - \kappa_{b}) I_{K-1}^{+} + K I_{K-1}^{-} - (2K+1) J_{K} \Big],$$
(2.2.46)

with integrals I_K^{\pm} and J_K defined by

$$I_{K}^{\pm} = \int_{0}^{\infty} \left[P_{a}^{*}(r)Q_{b}(r) \pm Q_{a}^{*}(r)P_{b}(r) \right] j_{K}\left(\frac{\omega r}{c}\right) \mathrm{d}r, \qquad (2.2.47)$$

$$J_{K} = \int_{0}^{\infty} \left[P_{a}^{*}(r) P_{b}(r) + Q_{a}^{*}(r) Q_{b}(r) \right] j_{K} \left(\frac{\omega r}{c} \right) \mathrm{d}r, \qquad (2.2.48)$$

where P(r) et Q(r) are respectively the large and small components of the radial part of the spin-orbitals and where $j_K(\frac{\omega r}{c})$ is a spherical Bessel function.

2.2.5 GRASP2018 code procedure

The GRASP2018 code (*General purpose Relativistic Atomic Structure Program* 2018) is a program to obtain the relativistic wavefunctions of an atomic system that implements the MCDHF method described above. It represents the most recent (Froese Fischer et al., 2019) and most powerful version of the relativistic atomic structure calculation programs originally developed by Grant et al. (1980). It consists of several modules that are used in a row.

Initially, after incorporating data concerning the nucleus of the element we aim to model in the RNUCLEUS program, the RCSFGENERATE program is supplied with a list of orbitals and configurations of interest in this model. The purpose is to generate the list of Configuration State Functions (CSFs). Then, to reduce the list of CSFs, we run RCSFINTERACT which is going to retain only CSFs that interact with CSFs of a reference list. Subsequently, the RANGULAR program is employed to compute a set of angular components required for the expression of the Hamiltonian matrix elements as defined in Eq. (2.2.21) and Eq. (2.2.24) (Grant, 2007), using the list of CSFs generated by the RCSFGENERATE program. Following this, the RWFNGENERATE program is used to generate the initial radial components. When executing this program, there are several options available. It is either possible to use a set of orbitals optimized in a previous calculation, or to use a set of spin-orbitals of the screened hydrogenic type, or also to generate a set of orbitals by means of a Thomas-Fermi potential (*e.g.* free electrons confined in a box).

Finally, the RMCDHF program is run in order to obtain the optimized spin-orbitals. For this purpose, the SCF method is used to iteratively solve the coupled MCDHF integro-differential equations by OL, EOL or EAL method described previously. This program calculates the radial interaction integrals but also different terms appearing in the MCDHF equations using initial radial parts generated by the RWFNGENERATE program. This step is repeated iteratively and stops when radial parts of the spin-orbitals have reached a certain convergence criterion. When the latter is satisfied, spin-orbitals are constructed from the optimized radial parts, and the CSFs are then given by Slater determinants constructed with these optimized spin-orbitals. To obtain the complete expression of the wavefunction for each ASF, the Hamiltonian matrix is assembled in the selected basis of CSFs. This matrix incorporates both diagonal and non-diagonal elements and is subsequently diagonalized to yield the energy levels and mixing coefficients for each ASF. The QED corrections aforementioned, are also included when RCI module is run. The corrected Hamiltonian is diagonalized again to obtain the corrected atomic energy levels and mixing coefficients. Finally, as a last step, a biorthonormal transformation is performed using the RBIOTRANSFORM module in order to gather and obtain an orthonormalized set of spin-orbitals that have been determined from separate RMCDHF runs for each parity. Finally,

RTRANSITION is run and gives transition probabilities, transition wavelengths and oscillator strengths involving all the atomic levels from the considered model.

In conclusion of this section, we provide a summary of the sequence followed, outlining the various modules employed throughout the calculation process.

RNUCLEUS	Generation nucleus data
RCSFGENERATE	Generation CSF lists
RCSFINTERACT	Reduce CSF list by retaining only CSF interacting with CSF of a reference list
RANGULAR	Generation of the angular parts
[↓] RWFNESTIMATE	Provides first estimates of radial parts
RMCDHF	Self-consistent field method (obtaining spin-orbitals)
RCI	Addition of relativistic corrections
↓ RBIOTRANSFORM	Biorthonormal transformation
\downarrow RTRANSITION	Generation of atomic parameters

2.3 Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT)

Configuration Interaction (CI) and Many-Body Perturbation Theory (MBPT) is an *ab initio* method used for high accuracy calculations initially developed by Dzuba et al. (1996). CI treats valence-valence correlations while MBPT describes valence-core and core-core correlations. It has been implemented in the AMBiT atomic structure code (Kahl and Berengut, 2019).

2.3.1 Configuration Interaction theory

The many-electron Hilbert space is separated into two subspaces \mathcal{P} and \mathcal{Q} . The first one, correspond to the *frozen core approximation* and the second one is complimentary to it and includes all the states with core excitations (Dzuba et al., 1996). The subspace \mathcal{Q} is treated using MBPT (Many-Body Perturbation Theory) since the projections of the wavefunctions associated with the lower-energy levels of the atom onto subspace \mathcal{Q} are relatively small. On the other hand, subspace \mathcal{P} is handled using the CI method (Configuration Interaction) since perturbation theory is not as effective within this subspace \mathcal{P} . The decomposition of the wavefunction in those subspaces depend on the definition of the core (*i.e.* definition of the number of electrons to be included in the core, N_{core}). It is also crucial to specify the one-particle wavefunctions for the core electrons, which must be eigenfunctions of the one-particle Hamiltonian expressed as outlined by Dzuba et al. (1996) as

$$h_0 \phi_i = \epsilon_i \phi_i. \tag{2.3.1}$$

We can use Slater determinants $|I\rangle$ of the functions ϕ_i as a basis set in the many-electron space. It is straightforward to determine the specific subspace to which a particular determinant $|I\rangle$ belongs. If all N_{core} of the lowest states are occupied in $|I\rangle$, then it pertains to the subspace \mathcal{P} otherwise, it belongs to the subspace \mathcal{Q} . We can define a projector to the subspace \mathcal{P} and \mathcal{Q} such that

1

$$\mathcal{P} = \sum_{I \in \mathcal{P}} |I\rangle \langle I| \text{ and } \mathcal{P} + \mathcal{Q} = 1.$$
 (2.3.2)

As the subspace \mathcal{P} is infinite-dimensional, it is impossible to find an exact solution of the Schrödinger equation in this subspace. Nonetheless, if the count of valence electrons is sufficiently low (less than three or four), it is possible to find a very good approximation with the CI method. This approach involves the introduction of a finite-dimensional model space $\mathcal{P}^{CI} \subset \mathcal{P}$ by defining the allowed configurations for the valence electrons. In the CI method, the atomic level wavefunctions ψ for a given total angular momentum and parity J π are then constructed as a linear combination of Slater determinants $|I\rangle$ (Dzuba et al., 1996):

$$\psi = \sum_{I \in \mathcal{P}^{CI}} C_I |I\rangle, \qquad (2.3.3)$$

where C_I are the coefficients obtained from the matrix eigenvalue problem of the CI Hamiltoninan:

$$\sum_{J \in \mathcal{P}^{CI}} H_{IJ} C_J = E C_I, \tag{2.3.4}$$

where H_{IJ} is the matrix element of the exact Dirac-Coulomb Hamiltonian operator projected on the model subspace using the projection operator \mathcal{P}^{CI} . As the core is frozen in the latter subspace, core electrons can be excluded by averaging the Hamiltonian over the single-determinant wavefunction of the core electrons:

$$\mathcal{H}^{CI} = \mathcal{P}^{CI} \mathcal{H} \mathcal{P}^{CI} = E_{\text{core}} + \sum_{i > N_{\text{core}}} h_i^{CI} + \sum_{j > i > N_{\text{core}}} \frac{1}{r_{ij}},$$
(2.3.5)

where E_{core} includes the kinetic energy of the core electrons and their Coulomb interaction with the nucleus and each other. The one-particle operator h_i^{CI} operates on the valence electrons and incorporates the kinetic term, the Coulomb interaction with the nucleus and the Coulomb interaction with the core electrons. The final term takes into consideration the interaction among the valence electrons themselves. We can rewrite Eq. (2.3.5) using \mathcal{P} instead of \mathcal{P}^{CI} as it is possible to choose \mathcal{P}^{CI} so that the accuracy of the solution of the Schrödinger equation in the \mathcal{P} subspace can be achieved:

$$\mathcal{H}^{CI} = \mathcal{P}\mathcal{H}\mathcal{P} = E_{\text{core}} + \sum_{i > N_{\text{core}}} h_i^{CI} + \sum_{j > i > N_{\text{core}}} \frac{1}{r_{ij}}.$$
(2.3.6)

2.3.2 Exact Hamiltonian expansion

Operator written in Eq. (2.3.6) can be used in Eq. (2.3.4) instead of \mathcal{H} . In this case determinants $|I\rangle$ and $|J\rangle$ only include the valence electrons. This corresponds to the pure CI method in the frozen-core approximation. To express the exact equivalent of the original Schrödinger equation within the subspace \mathcal{P} , we need to perform the \mathcal{P} - \mathcal{Q} decomposition of both the Hamiltonian and the wave function of the many-body problem (Dzuba et al., 1996; Berengut and Flambaum, 2006):

$$\mathcal{H}(\mathcal{P} + \mathcal{Q})\psi = E\psi,$$

$$\mathcal{H} = \mathcal{P}\mathcal{H}\mathcal{P} + \mathcal{P}\mathcal{H}\mathcal{Q} + \mathcal{Q}\mathcal{H}\mathcal{P} + \mathcal{Q}\mathcal{H}\mathcal{Q}.$$
 (2.3.7)

The Feshbach operator yields the exact energy when operating on the model function $\psi_P = \mathcal{P}\psi$. The Schrödinger equation can be written as:

$$\mathcal{PHP}\psi_P + \mathcal{PHQ}\psi_Q = E\psi_P \text{ and } \mathcal{QHP}\psi_P + \mathcal{QHQ}\psi_Q = E\psi_Q,$$
 (2.3.8)

where $\psi_Q = \mathcal{Q}\psi$. By eliminating ψ_Q , this gives us a Schrödinger-like equation in the subspace \mathcal{P} , with an energy-dependent effective Hamiltonian:

$$(\mathcal{PHP} + \Sigma(E))\psi_P = E\psi_P, \qquad (2.3.9)$$

where

$$\Sigma(E) = \mathcal{PHQ} \frac{1}{E - \mathcal{QHQ}} \mathcal{QHP}.$$
(2.3.10)

If the subspace \mathcal{P} includes only one electron the operator \mathcal{PHP} is reduced to the Dirac-Fock operator with the V^{N-1} potential that only includes the interaction among all the other N-1 electrons and Σ is reduced to the single-particle self-energy operator.

2.3.3 Many-body perturbation theory

Perturbation expansion of $\Sigma(E)$

In order to have a pertubation expansion for $\Sigma(E)$ it will depend on the choice of h_0 in Eq. (2.3.1). The simplest h_0 corresponds to the $V^{N_{\text{core}}}$ approximation, for which h_0 is the Dirac-Fock operator for the core. However, when we consider a atom with more than one valence electron, this approximation becomes too crude to start with. This implies that, in the self-consistent procedure, some or all of the valence electrons should also be incorporated. The one-electron Dirac-Fock operator in Eq. (2.3.1) is (Berengut and Flambaum, 2006):

$$h_0 = h_{DF} = c\vec{\alpha}.\vec{p} + (\beta - 1)c^2 - \frac{Z}{r} + V^{N_{DF}},$$
(2.3.11)

where $V^{N_{DF}}$ is the potential (both direct and exchange) of the N_{DF} electrons included in the self-consistent field Hartree-Fock procedure. It is important to note that N_{DF} electrons are not necessarily the number of electrons in the closed-shell core, as $N_{core} < N_{DF} < N$, where N is the total number of electrons. In the context of CI calculations, there are $N - N_{core}$ valence electrons. The remaining parameters such as α and β are Dirac matrices and the wavefunction can be written as

$$\psi(r) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa,m}(\hat{r})\\ iQ_{n\kappa}(r)\chi_{-\kappa,m}(\hat{r}) \end{pmatrix},$$
(2.3.12)

where $\kappa = (-1)^{j+l+1/2}(j+1/2)$ and $\chi_{\kappa,m}$, are the usual spherical spinors. The eigenvalue equation $h_{DF}\psi_i = \epsilon_i\psi_i$ can be written in the form of coupled ordinary differential equations (ODEs)

$$\frac{dP_i}{dr} = -\frac{\kappa}{r} P_i(r) + \frac{1}{c} \Big(\epsilon_i + \frac{Z}{r} - V^{N_{DF}} + 2c^2\Big) Q_i(r), \qquad (2.3.13)$$

$$\frac{dQ_i}{dr} = -\frac{1}{c} \left(\epsilon_i + \frac{Z}{r} - V^{N_{DF}}\right) P_i(r) + \frac{\kappa}{r} Q_i(r), \qquad (2.3.14)$$

for each orbital ψ_i . These ODEs can be solved numerically with some methods explained in Johnson (2007) .

In the CI space, the CSFs can also include valence-holes in otherwise filled shells, which can lie between the Fermi level of the system and some minimum n and l, the latter of which is referred as the frozen core. In this particle-hole (PH-CI) formalism, the CI Hamiltonian can be written as:

$$h_0 = h_{DF} = c\vec{\alpha}.\vec{p} + (\beta - 1)c^2 - \frac{Ze_i}{r_i} - e_i V^{N_{\text{core}}} + \sum_{i < j} \frac{e_i e_j}{|r_i - r_j|},$$
(2.3.15)

where $e_i = -1$ for valence electron states and +1 for holes. It is important to note that the onebody potential $V^{N_{\text{core}}}$ in the CI Hamiltonian only includes contributions from the core electrons since valence-valence correlations are included directly *via* the two-body Coulomb operator (Kahl and Berengut, 2019). To generate CSFs, a basis set of monoelectronic states $|i\rangle$ has to be built, that includes the core and valence states and a large number of virtual states. In the majority of the literature, they used B-splines basis set, formed by diagonalizing the Dirac-Fock operator on the basis set of B-splines and excluding orbitals with high energy. The large and small component $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ of the virtual orbitals are linear combinations of two sets of B-splines $\{l_i\}$ and $\{s_i\}$:

$$P_{n\kappa}(r) = \sum_{i} p_{i} l_{i}(r) \text{ and } Q_{n\kappa}(r) = \sum_{i} p_{i} s_{i}(r).$$
 (2.3.16)

Each component of the wavefunction has the same set of expansion coefficients, which are obtained variationally by solving the generalized eigenvalue problem (Johnson et al., 1988; Beloy and Derevianko, 2008):

$$Ap = \epsilon Sp, \tag{2.3.17}$$

where $A_{ij} = \langle i | h_{DF} | j \rangle$ is the matrix representation of the Dirac-Fock operator in the B-spline basis, $S_{ij} = \langle i | j \rangle$ is the overlap matrix, $|i\rangle = {l_i(r) \choose s_i(r)}$ are the B-spline basis functions and ϵ is the single particle energy of the virtual orbital. There is some freedom when choosing the exact values for the sets $\{l\}$ and $\{s\}$ as well as the boundary conditions of the resulting Bspline basis functions. The Dirac-Fock operator, h_{DF} is modified in order to take into account some corrections as the effects of finite nuclear size (Berengut et al., 2008), nuclear mass-shift (Berengut and Flambaum, 2006; Berengut, 2011) and the Breit interaction:

$$B_{ij} = -\frac{1}{2r_{ij}} (\alpha_i . \alpha_j + (\alpha_i . r_{ij})(\alpha_j . r_{ij})/r_{ij}^2).$$
(2.3.18)

The Lamb shift correction (calculated with the radiative potential method originally developed by (Flambaum and Ginges, 2005) is also considered in the Hamiltonian just as the self-energy and the vacuum polarization corrections (Ginges and Berengut, 2016a,b).

In order to do a perturbation expansion of Σ , let us define the single-particle Hamiltonian as:

$$h_{DF}a_i^{\dagger}|0\rangle = \epsilon_i a_i^{\dagger}|0\rangle \text{ with } \epsilon_i \equiv \langle i|h^{DF}|i\rangle,$$
 (2.3.19)

where operators a_i^{\dagger} and a_i are introduced to respectively create and annihilate a particle. The corresponding Dirac-Fock operator in the many-electron space, *i.e.* the many-body zero order Hamiltonian, can be written as

$$\mathcal{H}_0 = E_{\text{core}} + \sum_i \{a_i^{\dagger} a_i\} \epsilon_i, \qquad (2.3.20)$$

where the brackets denote normal ordering with respect to the closed-shell core. The exact Hamiltonian is written as:

$$\mathcal{H} = \sum_{i} h_{i}^{\text{nucl}} + \sum_{i < j} \frac{1}{r_{ij}},$$
(2.3.21)

where $h^{\text{nucl}} = c\vec{\alpha}.\vec{p} + (\beta - 1)m_ec^2 - Z/r_i$ can be separated into zero, one and two-body parts:

$$\mathcal{H}^{(0)} = E_{\text{core}},$$

$$\mathcal{H}^{(1)} = \sum_{ij} a_i^{\dagger} a_j \left[\langle i | h^{\text{nucl}} | j \rangle + \sum_m^{\text{core}} (\langle im | r_{12}^{-1} | jm \rangle - \langle im | r_{12}^{-1} | mj \rangle \right] = \sum_{ij} a_i^{\dagger} a_j \langle i | h^{CI} | j \rangle,$$

$$\mathcal{H}^{(2)} = \sum_{ijkl} a_i^{\dagger} a_j^{\dagger} a_l a_k \langle ij | r_{12}^{-1} | kl \rangle.$$
(2.3.22)

If one expands the Eq. (2.3.10) in the residual Coulomb interaction, $\mathcal{V} = \mathcal{H} - \mathcal{H}_0$, we obtain

$$\Sigma(E) = \mathcal{PHQ} \frac{1}{E - \mathcal{H}_0} \mathcal{QHP} + \mathcal{PHQ} \frac{1}{E - \mathcal{H}_0} \mathcal{QVQ} \frac{1}{E - \mathcal{H}_0} \mathcal{QHP} + \dots$$
(2.3.23)

One advantage of this formalism is that h_0 is not necessarily identical to h^{DF} . In principle, we have the flexibility to employ any set of functions in the virtual basis, provided that they maintain orthogonality. This necessitates that

$$\mathcal{V}^{(1)} = \langle i | h^{CI} - h_0 | j \rangle, \qquad (2.3.24)$$

has to be small. We can write Σ in matrix form such as

$$\Sigma_{IJ} = \sum_{M \in \mathcal{Q}} \frac{\langle I|H|M\rangle \langle M|H|J\rangle}{E - E_M} + \sum_{M,L \in \mathcal{Q}} \frac{\langle I|H|M\rangle \langle M|V|L\rangle \langle L|H|J\rangle}{(E - E_M)(E - E_L)} + \dots = (\Sigma_2)_{IJ} + (\Sigma_3)_{IJ} + \dots$$
(2.3.25)

where I and J enumerate determinants from the subspace \mathcal{P} , and M and L are determinants from the subspace \mathcal{Q} . In the literature, Σ is calculated to the second order of the perturbation expansion and shows for the one-valence-electron case, that this level of perturbation theory is sufficient to obtain accurante results (Berengut and Flambaum, 2006). Substituting Σ_2 into Eq. (2.3.9), we obtain the final matrix eigenvalue problem for the CI+MBPT technique:

$$\sum_{J \in \mathcal{P}} \left(H_{IJ} + \sum_{M \in \mathcal{Q}} \frac{\langle I | H | M \rangle \langle M | H | J \rangle}{E - E_M} \right) C_J = E C_I.$$
(2.3.26)

This method, CI+MBPT, includes the core-correlation effects by simply altering the matrix elements in the CI calculation.

Diagrammatic technique: MBPT corrections to valence-valence integrals

In previous implementations of CI+MBPT, Q space is defined to include all configurations with holes in the core. Now that we can include configurations with holes (PH-CI method) in the CI calculation, Q space has to be redefined. The PH-CI method introduces the possibility of an additional type of diagram that does not involve extra core holes but does include electron excitations beyond the valence space (Berengut, 2016). The number of terms in the MBPT corrections grows rapidly but the diagrammatic technique greatly simplifies the calculation of these terms (Dzuba et al., 1996). In this formalism, each contribution to the MBPT expansion is represented by a Goldstone diagram, with the number of external lines corresponding to the number of valence electrons included in the interaction (Berengut and Flambaum, 2006). At second order in the residual Coulomb interaction these valence-valence diagrams occur in the one-body, two-body, and effective three-body operators.

At the zero order of MBPT, we describe the interaction between valence electrons and the core using the two diagrams as shown in Figure 2.4. In these diagrams, summations for the internal lines run over the core. When considering the interaction with the Hartree-Fock field, the same diagrams apply, but the summations involve N^{DF} electrons. When the $N^{\text{core}} \ge N^{DF}$, there is a complete cancellation of these two contributions. This implies that all diagrams containing the elements shown in Figure 2.4 as one of their components vanish. The same principle applies to those blocks where one of the external electron lines is replaced by a hole line. In the case where $N^{\text{core}} < N^{DF}$, only a partial cancellation of the core-valence interaction and the Hartree-Fock field occurs. Consequently, the diagrams containing elements similar to those in Figure 2.4 persist, but the summations now run from $N^{\text{core}+1}$ to N^{DF} . These diagrams are termed *subtraction diagrams* because they arise from the stronger influence of the Hartree-Fock field in contrast to the core-valence interaction.



Figure 2.4: First-order diagrams for the valence electron interactions with the core (Dzuba et al., 1996)

Figure 2.5 shows an example of a one-body MBPT diagram describing the self-energy correction arising from core-valence interactions (left) and a subtraction diagram involving an interaction with an external field (right) (Dzuba et al., 1996). In these diagrams the external lines marked a, b, ... are valence electrons or holes, while the internal lines marked α , β are virtual electron orbitals outside the CI valence space. Diagrams with external field lines (such as at the right for Figure 2.5 and 2.6) are known as subtraction diagrams since the one-body external field operator is $h^{CI} - h^{DF}$. If $h^{CI} = h^{DF}$ these diagrams are then zero and cancelled each other. There are also three other one-valence-electron diagrams of Σ with their four subtraction diagrams that can be found in (Dzuba et al., 1996) and nine diagrams for the two-valence-electrons with four subtraction diagrams (an example is shown in Figure 2.6).



Figure 2.5: Example of some Goldstone diagrams describing a one-body core-valence correlation (left) and one-body subtraction diagram (right). Electrons are represented by lines running left to right, while lines running right to left are holes. $|a\rangle$ and $|b\rangle$ are valence orbitals, $|\alpha\rangle$ and $|\beta\rangle$ are virtual, and $|n\rangle$ is a hole in the core (Berengut and Flambaum, 2006)



Figure 2.6: Two-body valence-valence diagram (left) and valence-valence subtraction diagram (right). External lines a, b, c, d correspond to valence or hole orbitals in the CI subspace \mathcal{P} . Interior lines α and β are virtual electron orbitals.(Berengut, 2016).

Subtraction diagrams are partially cancelled out by some two- and three-body diagrams in the MBPT expansion (Berengut, 2011). Therefore, it is necessary to systematically incorporate all one-, two-, and three-body MBPT diagrams in the CI+MBPT procedure to ensure precise spectra. Despite this compensation, subtraction diagrams can become significant enough to be non-perturbative in open-shell systems, potentially impacting the accuracy of the resulting spectra (Berengut, 2011). As a result, there is a trade-off between generating more spectroscopic orbitals through calculations in a V^N potential and the potential presence of large subtraction diagrams when $V^{N_{DF}} \neq V^{N_{core}}$. The optimal choice will be contingent on the characteristics of the target system.

2.3.4 Emu CI

As explained above, the CI method relies on constructing and diagonalizing the Hamiltonian matrix over a set of many-electrons CSFs. The number of CSFs grows exponentially as we include a greater number of electrons within the CI problem subspace. Furthermore, it is worth noting that CI convergence is slow even for relatively straightforward systems with only a few valence electrons. This slow convergence makes it impractical to achieve saturation in openshell systems given the current computational time and memory limitations of supercomputers (Geddes et al., 2018).

To compensate the computational limits associated with CI calculations, a technique called *emu CI* (Dzuba et al., 2017) is employed. The term *emu* is used because the resulting CI matrix exhibits a resemblance to an emu's footprint. This approach is directly integrated into the AMBiT programs (Kahl and Berengut, 2019), ensuring that accuracy is maintained in the results (Geddes et al., 2018). This *emu CI* approach is particularly well-suited to the common case where only a few of the lowest-lying energy levels are calculated. In this strategy, the concept is that while higher-energy configurations contribute to the formation of lower-energy levels of interest, the impact of interactions among these higher-energy configurations on this contribution is relatively weak. Therefore, a complete CI matrix (as shown in Figure 2.7) is constructed with the matrix elements between these higher-energy CSFs deliberately set to zero. A CI matrix with fewer elements will require less memory and less time to diagonalize. In order to construct such a matrix, all important CSFs that contribute strongly to the low-energy levels of interest have to be situated on one side of the CI matrix. There are N_{small} lower-energy CSFs (interactions between these crucial CSFs, represented as the dark triangle in Figure 2.7 which is a real

and symmetric matrix), which are considered as the *small side* of the matrix. This small-side is created by permitting electron and/or hole excitations from a collection of leading configurations (which may not necessarily be the same as those used for the main CI-space) up to a specified maximum principal quantum number n and orbital angular momentum l. There are also interactions between higher-energy CSFs and lower-energy CSFs (represented by the lefthand rectangle in Figure 2.7 where N is considered as the *large side*) which will be included into the CI calculations since they have a significant impact on the lower-energy eigenstates. Conversely, interactions between one high-energy state and another high-energy state are expected to have negligible contributions to the overall CI wavefunction. Therefore, all interactions between higher-energy CSFs are set to zero (unshaded areas in Figure 2.7). Additionally, elements within the squares along the diagonal correspond to matrix elements between CSFs associated with the same relativistic configurations. Subsequently, the CI matrix can be assembled in such a way that the notable off-diagonal elements are clustered together in a block, leading to the structure represented in Figure 2.7.

The significant reduction in the number of non-zero elements within the *emu CI* matrix, compared to the standard CI matrix, leads to a substantial decrease in the computational resources required to accurately compute atomic spectra.



Figure 2.7: Schematic representation of the emu CI method, resembling an emu's footprint. The most crucial CSFs are located in the upper left corner, and the shaded regions constitute our effective CI matrix. Each square along the diagonal contains matrix elements between CSFs associated with the same relativistic configuration. The unshaded area symbolizes interactions between high-energy states, which are intentionally set to zero (Geddes et al., 2018).

The core-valence effects can be taken into account using MBPT as explained previously.

2.3.5 AMBiT package

The AMBiT software package (Kahl and Berengut, 2019) is designed to implement CI+MBPT for the comprehensive relativistic computation of atomic energy levels, as well as

electric and magnetic multipole transition matrix elements. Notably, the AMBiT software incorporates three-body MBPT corrections, resulting in a substantial improvement in accuracy, particularly for systems with several electrons. This capability enables the precise calculation of open-shell systems with a substantial number of valence electrons (N > 5) in a highly efficient computational manner. The CI+MBPT procedure can be performed in either the electron-only mode or in the particle-hole formalism (PH-CI) (Berengut and Flambaum, 2006). This adaptability enables the generation of open-shell configurations, characterized by partially occupied electron states. This can be achieved either by considering the entire electron population or by introducing an equivalent number of positively charged holes into an otherwise fully occupied shell. While both the electron-only and particle-hole approaches are theoretically equivalent within the CI framework, the particle-hole formalism offers a notable advantage. It allows for more precise Many-Body Perturbation Theory (MBPT) corrections by minimizing the impact of the so-called *subtraction diagrams* which can compromise accuracy in open-shell calculations. Furthermore, an emu CI approach has been incorporated into the traditional CI+MBPT method, as previously explained. This extension significantly reduces the computational complexity of CI+MBPT problems while preserving the accuracy of results.

Chapter 3

Atomic data obtained from pseudo- and fully-relativistic computational methods

In this chapter, we first detail the atomic computations for moderately-charged lanthanide ions (V–X) from Z = 57 to 62. We describe how the atomic data are obtained using HFR, MCDHF and CI+MBPT methods. After comparing theoretical results obtained with the different methods, we also provide a comparison between the available experimental data with our calculated theoretical values. Then, atomic data calculations for moderately-charged lanthanide ions (V–VII) from Z = 63 to 71 are also described and compared. For such elements (Eu to Lu), experimental values are only available for two ions, namely Yb V and Lu V and are compared with our theoretical values. Finally, we provide a detailed explanation about the ground state calculation for these elements with also a comparison with the available data in the literature.

3.1 Atomic structures for moderately-charged lanthanides from Z = 57 to 71

3.1.1 La V-X ions

In recent decades, various studies have been conducted on the lanthanum ions from La V to La X, employing spectral line observations to determine experimental energy levels. These investigations were performed using a variety of normal incidence and grazing incidence spectrographs while the sources used to excite the spectra were either traditional triggered sparks or laser-produced plasmas as the excitation sources.

For La V, 47 lines were registered by Epstein and Reader (1976) in the 389 - 825 Å wavelength region leading to the identification of 29 levels belonging to the $5s^25p^5$, $5s^25p^45d$, $5s^25p^46s$, and $5s5p^6$ configurations. In La VI, between 335 - 1 031 Å, there exists 103 lines that were identified by Gayasov et al. (1997) from the $5s^25p^4$ ground configuration to $5s^25p^35d$, $5s^25p^36s$, and $5s5p^5$ configurations, leading to the determination of 5 even- and 42 odd-parity levels. Concerning La VII, Gayasov et al. (1998) recorded 102 lines in the 307 - 1005 Å wavelength range. The latter were identified due to transitions from the 5 levels of the $5s^25p^3$ odd configuration to 37 levels of the $5s^25p^25d$, $5s^25p^26s$, and $5s5p^4$ even configurations. In 2008, Tauheed et al. (2008) established for La VIII all the 5 levels of the $5s^25p^2$ ground configuration and all the 26 levels belonging to the $5s^25p5d$, $5s^25p6s$, and $5s5p^3$ odd configurations thanks to the measurement of 71 lines between 280 - 1145 Å. In 2001, Churilov and Joshi (2001) classified 155

lines in the 363 – 870 Å region thanks to the analysis of complex transition arrays in La IX such as $(5p^3 + 5s5p5d + 4f5p^2 + 5s^26p + 5s^25f) - (5s5p^2, 5s4f5p + 5s^25d)$. This study completed the previous investigation of the La IX spectrum by Gayasov and Joshi (1998) who identified 49 lines belonging to the $(5s^25p + 5s^2 4f) (5s^25d + 5s^26s + 5s^25g + 5s5p^2 + 5s5p4f)$ transition arrays. These two last works enabled the determination of 64 odd levels and 35 even levels in La IX. Finally, Ryabtsev et al. (2002) analyzed the spectrum of La X listing 140 lines between 117 - 801 Å as being due to transitions from the $5s^2$, $5p^2$, 4f5p, 5s5d and 5s6s even configurations to the 5s5p, 5s6p, 5s5f, 5p5d, 4f5s and 4f5d odd configurations. This work allowed them to classify 24 and 40 energy levels in even- and odd-parities, respectively, confirming and extending the earlier study of Gayasov et al. (1999). Concerning the radiative decay rates for electric dipole transitions in those lanthanum ions, very few results were published so far. Only results for La IX and La X were published. In order to obtain radiative data as reliable as possible for those ions, we calculated atomic data for lanthanum ions using the three theoretical methods described in the previous chapter. After a comparison with the experimental data, a cross-check between the calculated data from these theoretical methods is done to assess the agreement between them.

We first used the pseudo-relativistic Hartree-Fock method described by Cowan (1981) to calculate the atomic structure and the radiative parameters. We do not include core-polarization (CPOL) effects in this work since we showed in Deprince et al. (2023) for uranium ions (U II and U III, which are analogous to the lanthanide ions Nd II and Nd III), that the opacity is lowered by a few percents in average as a result of the oscillator strength lowering due to core-polarization effects. As the lanthanide ions are similar to the actinides due to their complex configurations (actinides and lanthanides are characterized by a 5f and 4f unfilled subshell, respectively), the CPOL effects can be neglected for the ions of interest in this work, namely lanthanide ions, since these effects do not have a major impact on the opacities (Deprince et al., 2023). Moreover, CPOL effects becomes less important when the ionization degree is higher such as for the ions considered in this study.

We used a physical model in which valence-valence correlations are assumed to take place outside a Pd-like La XII ionic core. For this purpose, we introduced explicitly in the calculations the interacting configurations listed in Table 3.1. These configurations were chosen so that the most important valence-valence correlations outside the $4d^{10}$ subshell were considered.

While the spin-orbit parameters (ζ_{nl}) , calculated by the Blume-Watson method, were maintained at their *ab initio* values as advised by Cowan (1981), the radial Slater integrals corresponding to direct electrostatic interactions (F^k) , exchange electrostatic interactions (G^k) , and configuration interactions (R^k) were arbitrarily scaled down by a factor 0.90. In fact, Cowan (1981) proved that this process made it possible to artificially account for the impact of configurations that were not explicitly considered in the calculations in order to reduce the differences between the experimental energy levels, when known, and the calculated eigenvalues of the Hamiltonian.

LaV	LaVI	LaVII	LaVIII	LaIX	LaV
<u> </u>	La VI	Odd parity	La VIII Evon pority	Odd parity	La A Evon pority
So ² 5 n^5	$5c^25n^4$	$5c^2 5n^3$	$5c^2 5n^2$	So ² 5n	Even party $5c^2$
$58^{2}5p^{4}6p$	5°35°36°	$5s^{2}5n^{2}6n^{2}$	5s 5p	58 5p	505d
5s ⁻ 5p ⁻ 6p	5s ⁻ 5p [*] op	5s ⁻ 5p ⁻ 6p	5s-5pop	5s-op 5s ² 7#	5850 5864
5s ² 5p ² /p	5s ² 5p ³ /p	5s-5p-7p	5s-5p/p	5s ⁻ /p	5s6d
5s-5p-8p	5s-5p°8p	5s-5p-8p	58-5p8p	55-8p	5s/d
5s²5p*4f	$5s^{2}5p^{6}4f$	5s ² 5p ² 4f	5s ² 5p4f	5s ² 4f	5880
5s²5p³5f	5s²5p°5f	5s²5p²5f	Ss ² SpSf	5s²5f	5868
5s ² 5p ⁴ 6f	$5s^25p^36f$	5s ² 5p ² 6f	5s²5p6f	5s ² 6f	5s/s
5s ² 5p ⁴ 7f	5s ² 5p ³ 7f	5s ² 5p ² 7f	5s ² 5p7f	5s ² 7f	5s8s
5s ² 5p ⁴ 8f	5s ² 5p ³ 8f	5s ² 5p ² 8f	5s ² 5p8f	5s²8f	5s5g
$5s^25p^34f^2$	5s ² 5p ² 4f ²	5s ² 5p4f ²	$5s^24f^2$	5s5p5d	5s6g
$5s^25p^35d^2$	$5s^25p^25d^2$	5s ² 5p5d ²	$5s^25d^2$	5s5p6d	5s7g
$5s^25p^36s^2$	$5s^25p^26s^2$	5s ² 5p6s ²	$5s^26s^2$	5s5p7d	5s8g
$5s^25p^35d6s$	$5s^25p^25d6s$	5s ² 5p5d6s	$5s^25d6s$	5s5p8d	$5p^2$
5s5p ⁵ 5d	$5s5p^45d$	5s5p ³ 5d	5s5p ² 5d	5s5p6s	$5d^2$
5s5p ⁵ 6d	5s5p ⁴ 6d	5s5p ³ 6d	5s5p ² 6d	5s5p7s	$4f^2$
5s5p ⁵ 7d	5s5p ⁴ 7d	5s5p ³ 7d	5s5p ² 7d	5s5p8s	5р6р
5s5p ⁵ 8d	$5s5p^48d$	5s5p ³ 8d	5s5p ² 8d	5s4f5d	5p7p
5s5p ⁵ 6s	5s5p ⁴ 6s	5s5p ³ 6s	5s5p ² 6s	5s4f6d	5p8p
5s5p ⁵ 7s	5s5p ⁴ 7s	5s5p ³ 7s	5s5p ² 7s	5s4f7d	5p4f
5s5p ⁵ 8s	$5s5p^48s$	$5s5p^38s$	5s5p ² 8s	5s4f8d	5p6f
$5s5p^44f5d$	5s5p ³ 4f5d	5s5p ² 4f5d	5s5p4f5d	5s4f6s	5p7f
$5s5p^44f6d$	5s5p ³ 4f6d	$5s5p^24f6d$	5s5p4f6d	5s4f7s	5p8f
$5s5p^44f7d$	$5s5p^34f7d$	$5s5p^24f7d$	5s5p4f7d	5s4f8s	4f6p
$5s5p^44f8d$	$5s5p^34f8d$	$5s5p^24f8d$	5s5p4f8d	$5p^3$	4f7p
$5s5p^44f6s$	$5s5p^34f6s$	$5s5p^24f6s$	5s5p4f6s	$4f^3$	4f8p
$5s5p^44f7s$	$5s5p^{3}4f7s$	$5s5p^24f7s$	5s5p4f7s	$5\mathrm{p}4\mathrm{f}^2$	- 1
$5s5p^44f8s$	$5s5p^{3}4f8s$	$5s5p^24f8s$	5s5p4f8s	$5p^24f$	
$5p^44f^3$	$5n^6$	$5n^5$	$5n^4$	op ii	
$5p^{5}4f^{2}$	$5n^44f^2$	$5n^24f^3$	$5n4f^3$		
$5p^{6}4f$	$5p^{5}4f$	$5p^{3}4f^{2}$	$5p^{2}4f^{2}$		
59 11	SP II	$5p^{4}4f$	$5p^{-11}$ $5n^{3}4f$		
Erron noniter		Even nonita		Erron nonitre	
Even parity $5 - 25 - 46$	5 - 25 - 36	Even parity $5 - 25 - 26$	Odd parity $5x^25x^26x^2$	Even parity $5 - 2$	
$5s^{-}5p^{-}0s$	$5s^{2}5m^{3}7a$	$5s^{-}5p^{-}0s$	5s-5pos	$55^{-}05$	585p
5s-5p-7s	5s-5p*/s	5s-5p-7s	5s-5p/s	58-78 5-29-	5sop
5s-5p-8s	5s-5p°8s	5s-5p°8s	58-5p88	58-88	5s/p
5s²5p³5d	Ss ² Sp ⁹ Sd	5s ² 5p ² 5d	Ss ² SpSd	5s²5d	Ss8p
$5s^25p^46d$	$5s^25p^36d$	$5s^25p^26d$	5s ² 5p6d	$5s^26d$	5s4f
$5s^{2}5p^{4}/d$	$5s^{2}5p^{3}/d$	$5s^{2}5p^{2}/d$	$5s^25p/d$	$5s^{2}/d$	5851
5s ² 5p ⁴ 8d	$5s^25p^38d$	$5s^25p^28d$	5s ² 5p8d	5s ² 8d	5s6f
5s ² 5p ⁴ 5g	5s ² 5p ³ 5g	5s ² 5p ² 5g	5s ² 5p5g	5s ² 5g	5s7f
5s ² 5p ⁴ 6g	5s ² 5p ³ 6g	5s ² 5p ² 6g	5s ² 5p6g	5s ² 6g	5s8f
5s ² 5p ⁴ 7g	5s ² 5p ³ 7g	$5s^25p^27g$	5s ² 5p7g	5s ² 7g	5p5d
5s ² 5p ⁴ 8g	5s ² 5p ³ 8g	5s ² 5p ² 8g	5s ² 5p8g	5s-8g	5p6d
5s ² 5p ³ 4f5d	5s ² 5p ² 4f5d	5s ² 5p4f5d	5s ² 4f5d	5s5p ²	5p7d
5s ² 5p ³ 4f6s	$5s^25p^24f6s$	5s ² 5p4f6s	5s ² 4f6s	5s5p6p	5p8d
$5s5p^6$	5s5p ⁵	5s5p ⁴	5s5p ³	5s5p7p	5p6s
5s5p ⁵ 6p	5s5p ⁴ 6p	5s5p ³ 6p	5s5p ² 6p	5s5p8p	5p7s
5s5p ⁵ 7p	5s5p ⁴ 7p	5s5p ³ 7p	5s5p ² 7p	5s5p4f	5p8s
5s5p ⁵ 8p	5s5p ⁴ 8p	5s5p ³ 8p	5s5p ² 8p	5s5p5f	4f5d
$5s5p^54f$	$5s5p^44f$	5s5p ³ 4f	5s5p ² 4f	5s5p6f	4f6d
5s5p ⁵ 5f	5s5p ⁴ 5f	5s5p ³ 5f	5s5p ² 5f	5s5p7f	4f7d
5s5p ⁵ 6f	5s5p ⁴ 6f	5s5p ³ 6f	5s5p ² 6f	5s5p8f	4f8d
5s5p ⁵ 7f	5s5p ⁴ 7f	5s5p ³ 7f	5s5p ² 7f	$5s4f^2$	4f6s
5s5p ⁵ 8f	5s5p ⁴ 8f	5s5p ³ 8f	5s5p ² 8f	5s4f6p	4f7s
$5s5p^44f^2$	$5s5p^34f^2$	$5s5p^24f^2$	5s5p4f ²	5s4f7p	4f8s
5s5p ⁴ 4f6p	$5s5p^34f6p$	$5s5p^24f6p$	5s5p4f6p	5s4f8p	
$5s5p^44f7p$	$5s5p^34f7p$	$5s5p^24f7p$	5s5p4f7p	$5p^25d$	
$5s5p^44f8p$	$5s5p^34f8p$	$5s5p^24f8p$	5s5p4f8p	$4\hat{f}^25d$	
$5p^65d$	$5p^55d$	$5p^45d$	$5p^35d$	5p4f5d	
$5p^44f^25d$	$5p^44f5d$	$5p^24f^25d$	$5p4f^25d$	1	
$5p^54f5d$	· r · · · · ·	$5p^34f5d$	$5p^24f5d$		
-r		-r	-r		

Table 3.1: Configurations introduced in HFR calculations for La V–X ions.

Table 3.2 gives a summary of the number of levels and lines obtained with HFR method. An information about the ionization potential (IP) taken from the NIST database (Kramida et al., 2024) is also given since the HFR levels retained for the opacity computation were selected below this limit.

Table 3.2: Number of levels and transitions obtained in HFR calculations for La V–X ions. The ionization potentials are also given for each ion.

Ion	Number of levels ^a	Number of lines ^b	$IP (cm^{-1})^c$
La V	7 826	308 724	497 000
La VI	7 694	738 090	597 000
La VII	8 298	818 233	710 000
La VIII	3 974	749 088	847 000
La IX	1 001	86 088	960 000
La X	380	17 024	1 221 300

^a Total number of levels considered in HFR calculations.

^b Total number of transitions involving energy levels below the IP with HFR calculated $\log(qf)$ -values \geq -5.

^c Ionization potential taken from NIST (Kramida et al., 2024).

To evaluate the precision of the HFR atomic structure calculations, a preliminary analysis was conducted by comparing the results with existing experimental data. More specifically, when the computed wavelengths were compared to those measured by Epstein and Reader (1976) for La V, by Gayasov et al. (1997) for La VI, by Gayasov et al. (1998) for La VII, by Tauheed et al. (2008) for La VIII, by Gayasov and Joshi (1998) and Churilov and Joshi (2001) for La IX and by Ryabtsev et al. (2002) for La X, we found a good overall agreement, for which the average differences $\Delta\lambda/\lambda_{obs}$ (with $\Delta\lambda = \lambda_{HFR} - \lambda_{obs}$) were respectively equal to -0.055 ± 0.035 (La V), -0.054 ± 0.032 (La VI), -0.042 ± 0.018 (La VII), -0.037 ± 0.041 (La VIII), -0.010 ± 0.033 (La IX), and 0.005 ± 0.020 (La X). Figure 3.1 presents a comprehensive comparison between HFR calculations and the available experimental wavelengths for all the lanthanum ions examined in this section.



Figure 3.1: Deviation between HFR and observed wavelengths, $\Delta \lambda / \lambda_{obs}$ (with $\Delta \lambda = \lambda_{HFR} - \lambda_{obs}$) as a function of λ_{HFR} for spectral lines in La V–X ions. Experimental wavelengths are from Epstein and Reader (1976) for La V, by Gayasov et al. (1997) for La VI, by Gayasov et al. (1998) for La VII, by Tauheed et al. (2008) for La VIII, by Gayasov and Joshi (1998) and Churilov and Joshi (2001) for La IX and by Ryabtsev et al. (2002) for La X.

The second method used to obtain the radiative parameters is the fully-relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) method described by Grant (2007) implemented in the latest version of GRASP (General Relativistic Atomic Structure Program), *i.e.* GRASP2018 (Froese Fischer et al., 2019). For each of the lanthanum ions, a multi-reference

(MR) of spectroscopic configurations (representing physical orbitals directly involved in the transitions studied) was chosen. Then, different physical models were implemented in order to optimize the wavefunctions and the corresponding energy levels by gradually increasing the basis of configuration state functions (CSFs), thus taking into account more correlations. From this MR, the valence-valence (VV) and core-valence (CV) interactions were progressively built by adding single and double (SD) excitations to an active set of correlation orbitals (providing corrections to spectroscopic orbitals due to electronic correlations), as outlined in Table 3.3. In this table and from now on, the sets of active orbitals are denoted ns, n'p, n''d,... where n, n', n'',... are the maximum principal quantum numbers considered for each azimuthal quantum number l. In the case of La V–IX, orbitals 1s to 5p were optimized on the $5s^25p^k$ (k = 1-5) ground configuration while the 4f and 5d orbitals were optimized using the MR configurations, keeping all other orbitals fixed. For La X, orbitals 1s to 5s were optimized on the $5s^2$ ground configuration while the 5p, 5d and 4f orbitals were optimized on the MR. In the VV steps, only the new orbitals introduced (i.e. correlations orbitals) were optimized, the other ones being kept to their values obtained before. Finally, from the last valence-valence calculation (VV3), a CV model was built by adding SD excitations from the 4d core orbital to the VV1 valence orbitals, namely 5s, 5p, 5d, 5f and 5g. This last strategy led to extensive computations, as the total count of J-dependent configuration state functions (CSFs) ranged from several hundred thousand (La X) to more than four million (La V) when considering both parities together, as indicated in Table 3.3.

Calculation	La V	La VI	La VII	La VIII	La IX	La X
MR	Odd parity	Even parity	Odd parity	Even parity	Odd parity	Even parity
	$5s^25p^5$	$5s^25p^4$	$5s^25p^3$	$5s^25p^2$	5s ² 5p	$5s^2$
	5s ² 5p ⁴ 4f	5s ² 5p ³ 4f	5s ² 5p ² 4f	5s ² 5p4f	5s ² 4f	$5p^2$
	$5s^25p^34f^2$	$5s^25p^24f^2$	5s ² 5p4f ²	$5s^24f^2$	5s5p5d	5p4f
					5p ² 4f	5s5d
					5p4f ²	
					$5p^3$	
	Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity
	5s5p ⁶	5s5p ⁵	5s5p ⁴	5s5p ³	5s5p ²	5s5p
	5s5p ⁵ 4f	5s5p ⁴ 4f	5s5p ³ 4f	5s5p ² 4f	5s5p4f	5s4f
	5s ² 5p ⁴ 5d	5s ² 5p ³ 5d	5s ² 5p ² 5d	5s ² 5p5d	5s ² 5d	4f5d
					$5s4f^2$	5p5d
VV1	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}
VV2	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}
VV3	{7s,7p,7d,6f,5g}	{7s,7p,7d,6f,5g}	{7s,7p,7d,6f,5g}	{7s,7p,7d,6f,5g}	{7s,7p,7d,6f,5g}	{7s,7p,7d,6f,5g}
CV	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}
CSFs	4 389 357	3 707 264	2 084 541	839 430	1 222 461	271 640

Table 3.3: Computational strategies used in MCDHF calculations for La V–X ions.

A comparison of our MCDHF energy level values obtained in CV models with available experimental energy levels revealed a good agreement, the mean deviation $\Delta E/E_{\rm exp}$ (with $\Delta E = E_{\rm MCDHF} - E_{\rm exp}$) being found to be equal to 0.016 ± 0.005 (La V), 0.012 ± 0.019 (La VI), 0.020 ± 0.014 (La VII), -0.003 ± 0.021 (La VIII), -0.001 ± 0.011 (La IX), and 0.048 ± 0.050 (La X) when considering the experimental data reported by Epstein and Reader (1976), Gayasov et al. (1997, 1998), Tauheed et al. (2008), Gayasov and Joshi (1998), Churilov and Joshi (2001) and Ryabtsev et al. (2002).

The last theoretical method used was the Particule-Hole Configuration Interaction (PH-CI) method (Berengut and Flambaum, 2006) as implemented in the AMBiT package (Kahl and Berengut, 2019). This method was used for three specific ions, namely La V, La VIII and La X

In terms of AMBiT computations, they were predicated on the properties of the experimental energy levels that have been reported in the literature. Table 3.4 summarizes the various computational strategies that were used for the three ions in order to perform these calculations. The QED and Breit interactions were taken into account in all of the computations. In La V, the core spin-orbitals and the frozen core potential $V^{N_{core}}(r)$ were generated by solving the Dirac–Hartree–Fock (DHF) equations for the Cd-like ground configurations [Pd]5s² consisting in 48 electrons. The valence orbitals were determined by diagonalizing a set of *B*-splines using the DHF hamiltonian with the abovementioned frozen core potential. The emu CI expansions with symmetries as $J^{\pi} = 1/2^{\text{even}}-5/2^{\text{even}}$, $1/2^{\text{odd}}-3/2^{\text{odd}}$ were obtained by considering, for the large side, the single and double (SD) electron and hole excitations from the leading configurations, listed in Table 3.4, in which nl^{-k} stands for *k* holes in the *nl* shell to an active set of orbitals considered as inactive orbitals. For the small side, the active set of orbitals were reduced to {6s, 6p, 6d, 6f, 6g}. The dimensions (*N*) related to the large and small side are also given in the Table 3.4.

Regarding La VIII, the DHF equations were solved in a first step for the ground configuration of the Cd-like La X system, *i.e.* [Pd]5s², with 48 electrons in order to obtain the core orbitals. Then, this allowed to build the core electron potential $V^{N_{core}}(r)$ and to solve the frozen core DHF equations for the valence orbitals. The 57-electron wavefunction expansions in the emu CI step with symmetries as $J^{\pi} = 0^{\text{even}} - 2^{\text{even}}$, $0^{\text{odd}} - 3^{\text{odd}}$ were produced by taking into account, on the large side, all single and double electron and hole excitations from the leading configurations listed in Table 3.4 to the {22s, 22p, 22d, 22f, 22g} active set, while maintaining the inactive status of all core orbitals below 5s. The double electron and hole excitations were limited to the {12s, 12p, 12d, 12f, 12g} active set for the small side.

Lastly, the strategy for La X was the same as to the one used for La VIII, the leading configurations (as it can be seen in Table 3.4) and the multi-electron wavefunction symmetries being the only modifications. The latter being such that $J^{\pi} = 0^{\text{even}} - 5^{\text{even}}$, $0^{\text{odd}} - 6^{\text{odd}}$.

For each ion, the E1 line strengths, were calculated in the Babushkin gauge with photon frequencies $\omega = 0$ (*i.e.* in the non-relativistic limit) using our AMBiT models for the observed transitions reported by Epstein and Reader (1976), Tauheed et al. (2008) and Ryabtsev et al. (2002). The corresponding weighted oscillator strengths, gf, were determined afterward from the AMBiT S-values using the formula given below (Cowan, 1981) :

$$gf = 3.0376 \times 10^{-6} \sigma S, \tag{3.1.1}$$

where σ is the wavenumber (cm⁻¹) of the E1 transition as deduced from the AMBiT eigenvalues and S is the line strength (a.u).

Ions	La V	La VIII	La X
Leading configurations	$5p^{5}$	$5p^2$	$5s^{-0}$
	$5s^{-1}5p^{6}$	$5s^{-1}5p^3$	$5s^{-1}5p$
	$5p^44f$		$5s^{-1}4f$
	$5p^45d$		
	$5p^46s$		
Active set _{large side}	{12s, 12p, 12d, 12f, 12g}	{22s, 22p, 22d, 22f, 22g}	{22s, 22p, 22d, 22f, 22g}
Active set _{small side}	{6s, 6p, 6d, 6f, 6g}	{12s, 12p, 12d, 12f, 12g}	{12s, 12p, 12d, 12f, 12g}
N_{large}	3 959 094	611 676	49 763
$N_{\rm small}$	52 571	424 386	34 863

Table 3.4: Computational strategies used in emu CI calculations for La V, La VIII and La X ions.

Concerning La V, the relative differences, $\Delta E = (E_{\text{calculated}} - E_{\text{exp}})/E_{\text{exp}}$, with respect to the experimental energy levels published by Epstein and Reader (1976) ranged from less than -4% to 3% with an average of -0.4% and a standard deviation of 1.4%. For La VIII, the relative differences, ΔE , between our values and the available experimental energy levels (Tauheed et al., 2008) ranged from -5% to 4% with an average of 0.05% and a standard deviation of 2.4%. Finally, for La X, the relative differences with the experimental level energies of Ryabtsev et al. (2002) ranged from -4% to 2% with an average of -0.6% and a standard deviation of 1.1%.

We found a very good agreement between theoretical energy levels obtained by the three independent theoretical methods and the experimental energy levels available in the literature for each lanthanum ion. As these atomic data will be used in the determination of astrophysical opacities, it is therefore crucial to have the greatest number of spectral lines. The HFR method gives the highest number of lines compared to the two other theoretical methods since, in the former, we include much more spectroscopic configurations, *i.e.* between which transition parameters are determined. It is, thus, interesting to compare theoretical radiative data (such as oscillator strengths and transition probabilities) from this theoretical method with experimental data from the literature. Therefore, in Tables A.1 to A.6 in Appendix A, the HFR transition probabilities (qA) and oscillator strengths $(\log(qf))$ are listed for all experimentally observed lines published to date from the papers listed before for each lanthanum ion. We have compared these values with the gA-values previously calculated by Churilov and Joshi (2001) and Ryabtsev et al. (2002) for La IX and La X, respectively and were reported in the Table A.5 and A.6. Figure 3.2 provides additional illustration of this comparison, showing the ratio $qA_{\rm HFR}/qA_{\rm Previous}$ as a function of $gA_{\rm HFR}$. This figure shows that, although there are some notable discrepancies (larger than a factor of 2) between the two sets of results, overall agreement is fairly satisfactory. The average ratios for La IX and La X are 0.800 ± 0.756 and 0.791 ± 0.349 , respectively. While Churilov and Joshi (2001) and Ryabtsev et al. (2002) introduced a limited number of interacting configurations in their HFR calculations respectively for La IX and La X, it is reasonable to assume that our HFR results are more accurate than those previous published data.



Figure 3.2: Comparison between HFR transition probabilities (gA) and previously published values for experimentally observed lines in La IX and La X ions. For each ion, the ratio $gA_{HFR}/gA_{Previous}$ as a function of gA_{HFR} is shown. Previous data were taken from Churilov and Joshi (2001) for La IX and from Ryabtsev et al. (2002) for La X. The solid line corresponds to ratios equal to unity while the dotted lines correspond to deviations of a factor of 2.

We can also measure the accuracy of our HFR computations in the specific case of $5s^{2} {}^{1}S_{0}$ - 5s5p ^{1,3}P₁ transitions in La X for which Chou and Huang (1992), Curtis et al. (2000), and Biémont et al. (2000) calculated the radiative parameters. While the transition probabilities computed by Curtis et al. (2000) and Biémont et al. (2001) using the MCDHF approach show differences of 5-30 % from our qA-values, the oscillator strengths obtained by Chou and Huang (1992) using the multi-configuration relativistic random-phase approximation (MCRRPA) method were found to deviate by 10-25 % from our qf-values. We discovered that these data agreed fairly well with our conclusions. This is supported by the general good agreement we observed between the radiative parameters obtained for the entire set of lanthanum ions of interest in our work using the HFR, MCDHF and emu CI methods as it can be also seen in Table A.7 in Appendix A. Figures 3.3 and 3.4 display these comparisons. In fact, with reference to Figure 3.3, we can see that there is a good agreement between these theoretical values, with the majority of transitions in La V-X ions falling within the range of 30-35 %. In contrast, the mean deviation was found to be approximately 30 % when comparing HFR with emu CI for transitions in La V, La VIII, and La X ions as shown in Figure 3.4. However, in the latter, we notice some larger discrepancies between the different theoretical methods. These relate to a relatively small number of particular transitions whose line strength was found to be affected by significant cancellation effects. For instance, in Figure 3.4, it can be noticed, the three points that exhibit a significant deviation from the diagonal. They correspond to the transitions at $\lambda = 370.024$, 411.267 (La VIII), and 564.420 Å (La X) for which our HFR calculations yielded very small CFvalues of 0.003, 0.007, and 0.006, respectively, for the cancellation factor (CF). This suggests that the corresponding oscillator strengths were likely underestimated and should be used with caution. Nevertheless, opacity calculations which rely on the global accuracy of the atomic data used, should remain unchanged.



Figure 3.3: Comparison between oscillator strengths (log(gf)) computed in this work using HFR and MCDHF methods for experimentally observed lines in La V–X ions.



Figure 3.4: Comparison between oscillator strengths (log(gf)) computed in this work using HFR and emu CI (AMBiT) methods for experimentally observed lines in La V, La VIII and La X ions.

3.1.2 Ce V–X ions

There exists various studies concerning the spectra experimentally observed for cerium ions. The spectrum of Ce V, has been observed with a sliding-spark discharge and a 10.7 m normalincidence vacuum spectrograph. A total of 107 lines have been classified as transitions between 51 energy levels that belong to the configurations $5p^6$, $5p^54f$, $5p^55d$, $5p^56s$, $5p^56p$, and $5p^56d$. These lines are ranging between 365.661 - 2518.038 Å and were determined by Wajid et al. (2021). For Ce VI, 45 lines from $5s^25p^5 - (5s5p^6-5p^45d-5p^46s)$ ranging between 311.989 and 743.876 Å were classified by Churilov and Joshi (2000). Concerning Ce VII, the levels of three configurations, namely $5s^25p^4 - (5s5p^5 + 5p^36s)$ were identified by Tauheed and Joshi (2008) and also by Wajid and Jabeen (2019a), allowing the identification of 40 lines. Spectrum of Ce VIII was photographed by Wajid and Jabeen (2019b) using a spark source on a normal incident spectrograph and studied the ground and first excited configurations of this ions theoretically and experimentally. In this study, the ground state level of Ce VIII has been established for the first time. For the theoretical part, they used GRASP2018 package to calculate energy levels, wavelengths and transition rates for the $5s^25p^3$ and $5s5p^4$ configurations. They classified 24 lines coming from 13 levels of those configurations. For Ce IX, there is no experimental data published to date to our knowledge. Finally, the spectra of Ce X was investigated for the first time by Joshi et al. (2001) who could classified 34 lines in the 225 – 732 Å region coming from 8 odd-parity levels and 17 even-parity levels that belong to the configurations $5s^25p$, $5s^25d$, 5s²6s, 5s5p², 4f5s², 4f5s5p and 5s5p5d.

In this work, atomic data calculations were performed, as for the lanthanum ions, using the three theoretical methods mentioned before. First, we provide a detailed explanation of the HFR (Cowan, 1981) computations. For each cerium ion considered in the present study, a large number of configurations was included in the physical model as listed in Table 3.5

CeV	Ce VI	Ce VII	Ce VIII	Ce IX	Ce X
Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity
$5s^25p^6$	$5s^25p^5$	$5s^25p^4$	$5s^25p^3$	$5s^25p^2$	$5s^25p$
5s ² 5p ⁵ 6p	$5s^25p^46p$	5s ² 5p ³ 6p	$5s^25p^26p$	5s ² 5p6p	5s ² 6p
$5s^25p^57p$	$5s^25p^47p$	$5s^25p^37p$	$5s^25p^27p$	$5s^25p7p$	$5s^27p$
$5s^25p^58p$	$5s^25p^48p$	$5s^25p^38p$	$5s^25p^28p$	$5s^25p8p$	$5s^28p$
$5s^25p^54f$	$5s^25p^44f$	$5s^25p^34f$	$5s^25p^24f$	$5s^25p4f$	$5s^24f$
$5s^25p^55f$	$5s^25p^45f$	$5s^2 5p^3 5f$	$5s^25p^25f$	$5s^25p5f$	$5s^25f$
$5s^25p^56f$	$5s^25p^46f$	$5s^25p^36f$	$5s^25p^26f$	5s ² 5p6f	$5s^26f$
$5s^25p^57f$	$5s^25p^47f$	$5s^25p^37f$	$5s^25p^27f$	5s ² 5p7f	5s ² 7f
$5s^25p^58f$	$5s^25p^48f$	$5s^25p^38f$	$5s^25p^28f$	5s ² 5p8f	$5s^28f$
$5s^25p^44f^2$	$5s^25p^34f^2$	$5s^25p^24f^2$	$5s^25p4f^2$	$5s^24f^2$	5s5p5d
$5s^25p^45d^2$	$5s^25p^35d^2$	$5s^25p^25d^2$	$5s^25p5d^2$	$5s^25d^2$	5s5p6d
$5s^25p^46s^2$	$5s^25p^36s^2$	$5s^25p^26s^2$	$5s^25p6s^2$	$5s^26s^2$	5s5p7d
$5s^25p^45d6s$	$5s^25p^35d6s$	$5s^25p^25d6s$	5s ² 5p5d6s	$5s^25d6s$	5s5p8d
5s5p ⁶ 5d	5s5p ⁵ 5d	5s5p ⁴ 5d	5s5p ³ 5d	5s5p ² 5d	5s5p6s
5s5p ⁶ 6d	5s5p ⁵ 6d	$5s5p^46d$	5s5p ³ 6d	5s5p ² 6d	5s5p7s
5s5p ⁶ 7d	5s5p ⁵ 7d	5s5p ⁴ 7d	5s5p ³ 7d	5s5p ² 7d	5s5p8s
5s5p ⁶ 8d	$5s5p^58d$	$5s5p^48d$	5s5p ³ 8d	5s5p ² 8d	5s4f5d
5s5p ⁶ 6s	5s5p ⁵ 6s	5s5p ⁴ 6s	5s5p ³ 6s	5s5p ² 6s	5s4f6d
5s5p ⁶ 7s	5s5p ⁵ 7s	5s5p ⁴ 7s	5s5p ³ 7s	5s5p ² 7s	5s4f7d
5s5p ⁶ 8s	5s5p ⁵ 8s	5s5p ⁴ 8s	5s5p ³ 8s	5s5p ² 8s	5s4f8d
5s5p ⁵ 4f5d	5s5p ⁴ 4f5d	5s5p ³ 4f5d	5s5p ² 4f5d	5s5p4f5d	5s4f6s
5s5p ⁵ 4f6d	5s5p ⁴ 4f6d	5s5p ³ 4f6d	5s5p ² 4f6d	5s5p4f6d	5s4f7s
5s5p ⁵ 4f7d	5s5p ⁴ 4f7d	5s5p ³ 4f7d	5s5p ² 4f7d	5s5p4f7d	5s4f8s
5s5p ⁵ 4f8d	5s5p ⁴ 4f8d	5s5p ³ 4f8d	$5s5p^24f8d$	5s5p4f8d	5p ³
5s5p ⁵ 4f6s	5s5p ⁴ 4f6s	5s5p ³ 4f6s	5s5p ² 4f6s	5s5p4f6s	$4\bar{f}^3$
$5s5p^54f7s$	$5s5p^44f7s$	5s5p ³ 4f7s	$5s5p^24f7s$	5s5p4f7s	5p4f ²
5s5p ⁵ 4f8s	5s5p ⁴ 4f8s	5s5p ³ 4f8s	5s5p ² 4f8s	5s5p4f8s	5p ² 4f
$5p^54f^3$	$5p^44f^3$	$5p^6$	$5p^5$	$5p^4$	
$5p^64f^2$	$5p^54f^2$	$5p^44f^2$	$5p^24f^3$	5p4f ³	
	5p ⁶ 4f	$5p^54f$	$5p^34f^2$	$5p^24f^2$	
			$5p^44f$	5p ³ 4f	
Odd parity	Even parity	Odd parity	Even parity	Odd parity	Even parity
$5s^25p^56s$	$5s^25p^46s$	5s ² 5p ³ 6s	5s ² 5p ² 6s	5s ² 5p6s	$5s^26s$
$5s^25p^57s$	$5s^25p^47s$	5s²5p³7s	$5s^25p^27s$	5s²5p7s	$5s^27s$
$5s^25p^58s$	$5s^25p^48s$	5s ² 5p ³ 8s	5s ² 5p ³ 8s	5s²5p8s	$5s^28s$
$5s^25p^55d$	$5s^25p^45d$	5s ² 5p ³ 5d	$5s^25p^25d$	5s ² 5p5d	$5s^25d$
$5s^25p^56d$	$5s^25p^46d$	$5s^25p^36d$	$5s^25p^26d$	5s ² 5p6d	$5s^26d$
$5s^25p^57d$	$5s^25p^47d$	$5s^25p^37d$	$5s^25p^27d$	$5s^25p7d$	$5s^27d$
$5s^25p^58d$	$5s^25p^48d$	$5s^25p^38d$	$5s^25p^28d$	5s ² 5p8d	$5s^28d$
$5s^25p^55g$	$5s^25p^45g$	5s ² 5p ³ 5g	$5s^25p^25g$	5s ² 5p5g	5s ² 5g
$5s^25p^56g$	$5s^25p^46g$	5s ² 5p ³ 6g	5s ² 5p ² 6g	5s ² 5p6g	5s ² 6g
$5s^25p^57g$	$5s^25p^47g$	$5s^25p^37g$	$5s^25p^27g$	5s ² 5p7g	$5s^27g$
5s ² 5p ⁵ 8g	5s ² 5p ⁴ 8g	5s ² 5p ³ 8g	5s ² 5p ² 8g	5s ² 5p8g	5s ² 8g
5s ² 5p ⁴ 4f5d	5s ² 5p ³ 4f5d	$5s^25p^24f5d$	5s ² 5p4f5d	5s ² 4f5d	$5s5p^2$
$5s^25p^44f6s$	5s ² 5p ³ 4f6s	$5s^25p^24f6s$	5s ² 5p4f6s	$5s^24f6s$	5s5p6p
5s5p ⁶ 6p	5s5p ⁶	5s5p ⁵	5s5p ⁴	5s5p ³	5s5p7p
5s5p ⁶ 7p	5s5p ⁵ 6p	5s5p ⁴ 6p	5s5p ³ 6p	5s5p ² 6p	5s5p8p
5s5p ⁶ 8p	5s5p ⁵ 7p	5s5p ⁴ 7p	5s5p ³ 7p	5s5p ² 7p	5s5p4f
5s5p ⁶ 4f	5s5p ⁵ 8p	5s5p ⁴ 8p	5s5p ³ 8p	5s5p ² 8p	5s5p5f
5s5p ⁶ 5f	5s5p ⁵ 4f	5s5p ⁴ 4f	5s5p ³ 4f	5s5p ² 4f	5s5p6f
5s5p ⁶ 6f	5s5p ⁵ 5f	5s5p ⁴ 5f	5s5p ³ 5f	5s5p ² 5f	5s5p7f
5s5p ⁶ 7f	5s5p ⁵ 6f	5s5p ⁴ 6f	5s5p ³ 6f	5s5p ² 6f	5s5p8f
5s5p ⁶ 8f	$5s5p^{5}7f$	5s5p ⁴ 7f	5s5p ³ 7f	5s5p ² 7f	$5s4f^2$
$5s5p^54f^2$	5s5p ⁵ 8f	5s5p ⁴ 8f	5s5p ³ 8f	5s5p ² 8f	5s4f6p
5s5p ⁵ 4f6p	$5s5p^44f^2$	$5s5p^34f^2$	$5s5p^24f^2$	5s5p4f ²	5s4f7p
5s5p ⁵ 4f7p	5s5p ⁴ 4f6p	5s5p ³ 4f6p	5s5p ² 4f6p	5s5p4f6p	5s4f8p
5s5p ⁵ 4f8p	5s5p ⁴ 4f7p	5s5p ³ 4f7p	5s5p ² 4f7p	5s5p4f7p	$5p^25d$
$5p^54f^25d$	5s5p ⁴ 4f8p	5s5p ³ 4f8p	5s5p ² 4f8p	5s5p4f8p	4f ² 5d
5p ⁶ 4f5d	5p ⁶ 5d	5p ⁵ 5d	5p ⁴ 5d	$5p^35d$	5p4f5d
	$5p^44f^25d$	5p ⁴ 4f5d	$5p^24f^25d$	5p4f ² 5d	
	5p ⁵ 4f5d		5p ³ 4f5d	5p ² 4f5d	

Table 3.5: Configurations included in HFR calculations for Ce V–X ions.

Table 3.6 summarizes the number of levels and transitions obtained using this method considered in opacity calculations. IP from NIST database (Kramida et al., 2024) are also mentioned since the calculated levels selected for opacity calculations are below those IPs.

Table 3.6: Ionization potentials, number of levels and number of spectral lines included in the opacity calculations for Ce V–X ions.

Ion	Number of levels ^{<i>a</i>}	IP $(\mathrm{cm}^{-1})^b$	Number of lines ^c
Ce V	3 444	528 700	131 248
Ce VI	7 826	626 000	657 090
Ce VII	7 694	734 000	918 542
Ce VIII	8 298	855 000	1 113 548
Ce IX	3 974	1 008 000	834 383
Ce X	1 001	1 129 000	99 259

^a Total number of HFR levels considered in opacity calculations

^b Ionization potential from NIST atomic database (Kramida et al., 2024)

^c Total number of transitions involving energy levels below the IP with HFR calculated $\log(qf)$ -values \geq -5.

One way to assess the accuracy of the atomic structures obtained using the HFR method is to look at the good overall agreement (to within a few percent) between the wavelengths measured in the laboratory and those calculated. Indeed, it was found that the average relative difference $\Delta\lambda/\lambda_{Obs}$ (with $\Delta\lambda = \lambda_{HFR} - \lambda_{Obs}$) was equal to 0.028 ± 0.081 (Ce V), -0.063 ± 0.023 (Ce VI), -0.044 ± 0.019 (Ce VII), -0.034 ± 0.045 (Ce VIII) and -0.011 ± 0.015 (Ce X) when considering the experimental wavelengths published by Churilov and Joshi (2000), Joshi et al. (2001), Tauheed and Joshi (2008), Wajid and Jabeen (2019a,b) and Wajid et al. (2021). It is however interesting to note that the biggest deviations (roughly 25%) were found for a small number of Ce V lines between 507 and 537 Å. These lines were all related to $5s^25p^54f - 5s5p^64f$ transitions, for which it was exceedingly difficult to theoretically reproduce the observed wavelengths. This was primarily because both configurations involved in these transitions seemed to be heavily influenced by other configurations, $5s^25p^6$, $5s^25p^44f^2$, $5s^25p^45d^2$, $5s^5p^54f^25d$, $5p^54f^25d$, $5p^54f^3$ for the lower even-parity one, and $5s^25p^55d$, $5s^25p^44f^2$, $5s^5p^54f^2$, $5p^54f^25d$, $5p^64f5d$ for the upper odd-parity one. Figure 3.5 presents a comprehensive comparison of HFR with available experimental wavelengths for all cerium ions taken into consideration in this work.


Figure 3.5: Deviation between HFR and observed wavelengths, $\Delta \lambda / \lambda_{Obs}$ (with $\Delta \lambda = \lambda_{HFR} - \lambda_{Obs}$) as a function of λ_{HFR} for spectral lines in Ce V, Ce VI, Ce VII, Ce VIII and Ce X ions.

We also used the two other independent theoretical approaches, the purely relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) (Grant, 2007) and the Particle-Hole Configuration Interaction (PH-CI) (Berengut, 2016) methods, as for La ions, to further evaluate the accuracy of the HFR results. More specifically, the radiative parameters and atomic structures of three

distinct cerium ions (Ce V, Ce VIII, and Ce X) were determined using those techniques.

Concerning the MCDHF method, for each cerium ion, a MR of spectroscopic configurations was chosen. From this MR, as for La ions, we built VV and CV interactions by adding progressively SD excitations as summarized in Table 3.7. In the case of Ce V, orbitals 1s to 5p were optimized on the $5s^25p^6$ ground configuration while the 4f and 5d orbitals were optimized using the MR configurations, keeping all other orbitals fixed. A first valence-valence model (VV1) was built by adding to the MR configurations, single and double (SD) excitations from 5s, 5p, 5d and 4f to VV1 active orbitals. In this step, only the new orbitals, 5f and 5g, were optimized, the other ones being kept to their values obtained before. The same strategy was used to build a more elaborate VV model, namely VV2, by considering the additional set of 6s, 6p, 6d, 6f and 5g active orbitals. From the latter calculation, a CV model was then built by adding SD excitations from the 4d core orbital to the MR valence orbitals, namely 5s, 5p, 5d, and 4f. This gave rise to a total of 862 213 and 675 385 *J*-dependent configuration state functions for the even- and odd-parities, respectively.

For Ce VIII, VV and CV models were then built using exactly the same strategy as the one followed in the case of Ce V. CV computations lead to the consideration of 328 029 and 716 638 configuration state functions in the calculations within the odd- and even-parities, respectively.

Finally, for Ce X, configurations listed in Table 3.7 were considered to build the MR. From this MR, the above mentioned VV1 and VV2 models were added by a VV3 model in which the active set included 7s, 7p, 7d, 6f and 5g orbitals. From the latter VV3 model, CV calculations were then carried out by allowing SD excitations from the 4d core orbital to 5s, 5p, 5d, 4f, 5f and 5g, giving rise to 849 798 and 372 663 configuration state functions in the odd- and even-parities, respectively.

Calculation	Ce V	Ce VIII	Ce X
MR	Even parity	Odd parity	Odd parity
	$5s^25p^6$	$5s^25p^3$	5s ² 5p
	$5s^25p^54f$	$5s^25p^24f$	$5s^24f$
	$5s^25p^44f^2$	$5s^25p4f^2$	5s5p5d
	$5s5p^65d$	$5p^5$	5p ² 4f
	$5p^64f^2$	5s5p ³ 5d	$5p4f^2$
		$5p^44f$	$5p^3$
	Odd parity	Even parity	Even parity
	5s5p ⁶ 4f	$5s5p^4$	5s5p ²
	$5s^25p^55d$	5s5p ³ 4f	5s5p4f
	$5s5p^54f^2$	$5s^25p^25d$	$5s^25d$
		$5s5p^24f^2$	$5s4f^2$
VV1	{5s,5p,5d,5f,5g}	$\{5s, 5p, 5d, 5f, 5g\}$	{5s,5p,5d,5f,5g}
VV2	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}
VV3			{7s,7p,7d,6f,5g}
CV	{5s,5p,5d,4f}	{5s,5p,5d,4f}	{5s,5p,5d,5f,5g}
CSFs	1 537 598	1 044 667	1 222 461

Table 3.7: Computational strategies used in MCDHF calculations for Ce V, Ce VIII and Ce X ions.

The mean deviation $\Delta E/E_{exp}$ was found to be equal to 0.059 \pm 0.049 (Ce V), -0.012 \pm 0.014 (Ce VIII), and -0.001 \pm 0.015 (Ce X) when taking into account the experimental data reported by Wajid et al. (2021), Wajid and Jabeen (2019b), and Joshi et al. (2001), respectively. This comparison between our MCDHF energy level values obtained in CV models and available experimental energy levels revealed a good agreement.

Finally, we applied the PH-CI method and more particularly the emu CI approach (Geddes et al., 2018) in order to calculate the atomic data for Ce ions. Calculations have primarily focused on the characteristics of the experimental energy levels reported in the literature as listed in the beginning of this section. In all the calculations for each cerium ion, the Breit and QED interactions have been included.

In order to perform emu CI calculations, different computation strategies have been employed for the three ions. A model similar to the one used for Ne-like Fe XVI by Kuhn et al. (2020) has been applied to Ce V. Specifically, the DHF equations for the Xe-like ground configurations [Pd] $5s^25p^6$ with 54 electrons have been solved, yielding the core spin-orbitals and the frozen core potential $V^{N_{\text{core}}}(r)$. By diagonalizing a set of *B*-splines with the aforementioned frozen core potential and the DHF hamiltonian, the valence orbitals have been determined. The emu CI expansions with symmetries as $J^{\pi} = 0^{\text{even}} - 5^{\text{even}}$, $0^{\text{odd}} - 4^{\text{odd}}$ have been obtained by considering for the large side the SD electron and hole excitations from this leading configurations, namely $5p^{6}$, $5p^{-1}4f$, $5p^{-1}5d$, $5p^{-1}6s$, $5p^{-1}6p$, $5p^{-1}6d$ to the active set of orbitals {10s, 10p, 10d, 10f, 10g} with all the core orbitals lower than 5s inactive, *i.e.* 5s to 10s, 5p to 10p, 5d to 10d, 4f to 10f and 5g to 10g. For the small side, the active set of orbitals were reduced to {6s, 6p, 6d, 6f, 6g}, SD electron only excitations have been considered and the leading configurations set were extended by adding $5p^{-2}4f^2$, $5s^{-1}5p^{-1}4f^2$, $5s^{-2}4f^2$, $5p^{-2}4f5d$, $5s^{-1}5p^{-1}4f5d$, $5s^{-2}4f5d$. The resulting emu CI matrix dimensions were N = 6.651.739 for the large side and $N_{\text{small}} = 13.819$ for the small side. Wajid et al. (2021) published experimental energy levels that have agreements ranging from less than 1% to 2%, with the exception of the $5p^{-1}4f$ even levels, where the agreements were around 8 %.

Concerning Ce VIII, the DHF equations have been solved with 48 electrons in order to obtain the core orbitals for the ground configuration of the Cd-like Ce XI system, *i.e.* [Pd]5s². This allowed us to solve the frozen core DHF equations for the valence orbitals and construct the core electron potential $V^{N_{\text{core}}}(r)$ in a second step. The 51-electron wavefunction expansions in the emu CI step with symmetries as $J^{\pi} = 1/2^{\text{even}} - 5/2^{\text{even}}$, $1/2^{\text{odd}} - 5/2^{\text{odd}}$ were produced by taking into account, for the large side, all SD electron and hole excitations from the $5p^2$ and $5s^{-1}5p^3$ leading configurations to {22s, 22p, 22d, 22f, 22g} maintaining all core orbitals below 5s as inactive. For the small side, the double electron and hole excitations have been restricted to the {12s, 12p, 12d, 12f, 12g} active set. For the large side, the corresponding dimensions were N = 1 146 875, and for the small side, they were $N_{\text{small}} = 513$ 545. Our eigenvalues differed by less than 1% to 2.4% from the available experimental energy levels (Wajid and Jabeen, 2019b).

Lastly, the approach for Ce X was essentially the same as the one for Ce VIII, with the exception of the multielectron wavefunction symmetries and leading configurations. These were respectively 5p, $5s^{-1}5p^2$ and 4f with symmetries such as $J^{\pi} = 1/2^{\text{even}} - 9/2^{\text{even}}$, $1/2^{\text{odd}} - 7/2^{\text{odd}}$. The dimensions of the emu CI large and small sides were N = 577246 and $N_{\text{small}} = 53973$, respectively. The level energies were in accordance with the experimental ones from Joshi et al. (2001) and ranged from less than 1% to 5%, except for the 4f ${}^2F_{5/2,7/2}^0$ doublet, where it was

roughly 19%.

At this stage, atomic data calculations were performed and energy levels were compared between these three independent theoretical methods and the data available in the literature. As we mentioned earlier, HFR method gave the greatest number of lines compared to the two other theoretical methods as we included much more spectroscopic configurations. It is, thus, interesting, such as for the La ions, to compare theoretical wavelengths and radiative data from HFR method such as oscillator strengths and transitions probabilities with experimental data from the literature when they are available.

Tables B.1 to B.5 in Appendix B contain a summary of the oscillator strengths $(\log(qf))$ and transition probabilities (qA) obtained by the HFR theoretical approach for all experimentally observed lines in Ce V, Ce VI, Ce VII, Ce VIII, and Ce X. When available, we also include previously published data for gA- and/or $\log(gf)$ -values in the same tables. These data were taken from the works of Wajid et al. (2021) for Ce V, Churilov and Joshi (2000) for Ce VI, Wajid and Jabeen (2019a) for Ce VII, Wajid and Jabeen (2019b) for Ce VIII, and Joshi et al. (2001) for Ce X. The comparison between both sets of results is illustrated in Figure 3.6 where the ratio $qA_{\rm HFR}/qA_{\rm Previous}$ is shown as a function of $qA_{\rm HFR}$ for all the experimentally observed lines in cerium ions. Examining this figure reveals that for the vast majority of the transitions in each ion, there is a reasonably good overall agreement (within a factor of two). Upon closer examination, we found that, in the case of Ce VII, Ce VIII, and Ce X ions, there is a much better agreement (of the order of 25% on average with a much smaller dispersion in the discrepancies). This can be explained by the fact that our HFR calculations for Ce V and Ce VI ions were based on far more complex physical models than the theoretical studies previously published by Wajid et al. (2021) and Churilov and Joshi (2000), who included fewer interacting configurations in their HFR calculations. However, the radiative parameters for Ce VII, Ce VIII, and Ce X ions, as reported by Wajid and Jabeen (2019a), Wajid and Jabeen (2019b) and Joshi et al. (2001), were derived from more comprehensive theoretical frameworks. Indeed, Wajid and Jabeen employed the purely relativistic multi-configurational Dirac-Fock (MCDF) method in the cases of Ce VII and Ce VIII, accounting for numerous valence-valence and core-valence interactions up to n = 8 from the MR 5s²5p⁴, 5s5p⁵ and 5s²5p³, 5s5p⁴, 5s²5p²5d, and 5s²5p²6s, respectively. Joshi et al. (2001) used a less comprehensive set of HFR calculations for Ce X, but even so, by including 13 odd-parity and 12 even-parity configurations in their model, they were able to account for the most significant valence-valence correlation effects. This ion, with a $5s^25p$ ground configuration, has a simpler electronic structure than those that characterize lower ionization stages of cerium atoms. Therefore, we can draw the conclusion that our work's oscillator strengths and transition probabilities using the HFR method agree better with the few most trustworthy results that have been published in the past for cerium ions of interest.



Figure 3.6: Comparison between HFR transition probabilities (gA) and previously published values for experimentally observed lines in Ce V, Ce VI, Ce VII, Ce VIII and Ce X ions. For each ion, the ratio $gA_{HFR} / gA_{Previous}$ is shown as a function of gA_{HFR} . The dashed lines correspond to ratios equal to unity while the dotted lines correspond to deviations of a factor of two.

In order to assess the precision of our HFR computations, we additionally compared them with the radiative parameters that we obtained through our research by employing the MCDHF and AMBiT approaches for Ce V, Ce VIII, and Ce X ions. For experimentally observed lines in these ions, such comparisons are reported in Table B.6 in Appendix B. Figures 3.7 and 3.8, which show our log(gf)-values computed with HFR as a function of the ones obtained with MCDHF and emu CI (AMBiT), respectively, further illustrate these comparisons. Upon examining this table and these two figures, it is interesting to note that there is a strong agreement between the three theoretical approaches. In particular, when comparing the HFR gf-values for the entire set of transitions listed in Table B.6 to the MCDHF and AMBiT results, we found that, they show relative differences of roughly 40% and 35% on average respectively. If we limit our analysis to

the most intense lines with $\log(gf) \ge -2$, these deviations drop to 35% and 30%, respectively. Based on all of these factors, we can conclude that the radiative parameters, computed with HFR method, obtained in this work constitute a trustworthy data set that we can use to calculate the opacity of interest when modeling kilonova spectra.



Figure 3.7: Comparison between oscillator strengths (log(gf)) computed in this work using HFR and MCDHF methods for experimentally observed lines in Ce V, Ce VIII and Ce X ions.



Figure 3.8: Comparison between oscillator strengths (log(gf)) computed in this work using HFR and emu CI (AMBiT) methods for experimentally observed lines in Ce V, Ce VIII and Ce X ions.

Concerning experimental considerations for moderately-charged Pr ions, spectral lines and energy levels were only reported for Pr V and Pr X. More specifically, in the case of Pr V, 12 transitions were classified in the region $840 - 2\ 250$ Å by Kaufman and Sugar (1967), which enabled to identify the 8 levels belonging to the 5p⁶4f, 5p⁶5d, 5p⁶6s, 5p⁶6p and 5p⁶7s configurations. Regarding Pr X, Bekker et al. (2019) measured optical inter-configuration lines using the Heidelberg electron beam ion trap (HD-EBIT), identifying the 5p–4f orbital crossing and, as a result, determining the frequency of 5p² ³P₀ – 5p4f ³G₀ clock transition with enough accuracy for ultra-high resolution quantum-logic spectroscopy. The experimental determination of 15 energy levels was made possible by the observation of 22 forbidden lines in the 5p² and 5p4f configurations in the latter work.

Theoretically, a few radiative parameter computations were released for a restricted set of electric dipole transitions. For Pr V, Karacoban and Dogan (2015) used the relativistic Hartree-Fock (HFR) method to calculate the oscillator strengths and transition probabilities for the 12 lines observed experimentally by Kaufman and Sugar (1967). The findings of this work were found to be in general good agreement with the previous data computed for the same transitions by Migdalek and Baylis (1979) using the relativistic single-configuration Hartree-Fock method, by Migdalek and Wyrozumska (1987) by means of different versions of the relativistic model potential approach, by Savukov et al. (2003) using the relativistic many-body perturbation theory, and by Zilitis (2014) using the Dirac-Fock method. Other studies about oscillator strength calculations were published on the one hand by Glushkov (1992) and Zilitis (2014) using the relativistic model, respectively, for some resonance transitions involving low-lying configurations along the Cs isoelectronic sequence, including Pr V and on the other hand, by Cheng and Froese Fischer (1983) using term-dependent Hartree-Fock technique for the $4d^{10} - 4d^9nf$ ¹P transitions in Xe-like ions, including Pr VI.

In order to compute the atomic structure of such ions, we used the same procedure as we did in the two previous sections, namely for La and Ce ions. The first theoretical method used is the HFR introduced by Cowan (1981). For each ion, the HFR physical model retained was based, as for La and Ce ions, on a Pd-like ionic core with 46 electrons filling all the subshells up to $4d^{10}$ surrounded by k valence electrons, with k ranging from 4 to 9, depending on the total number of electrons in the atomic system. As for the intravalence correlations, they were evaluated by introducing explicitly a large number of interacting configurations listed in Table 3.8.

Among the six ions considered in this section, only Pr V has experimentally measured wavelengths for electric dipole transitions Kaufman and Sugar (1967). When comparing our HFR values with these experimental data, we found a good overall agreement, the average differences $\Delta \lambda / \lambda_{Obs}$ (with $\Delta \lambda = \lambda_{HFR} - \lambda_{Obs}$) being found to be equal to 0.011 ± 0.042.

Pr V	Pr VI	Pr VII	Pr VIII	Pr IX	Pr X
Odd parity	Even parity	Odd parity	Even parity	Odd parity	Even parity
5s ² 5p ⁶ 4f	$5s^25p^6$	$5s^25p^5$	$5s^25p^4$	$5s^25p^3$	$5s^25p^2$
5s ² 5p ⁶ 5f	5s ² 5p ⁵ 6p	5s ² 5p ⁴ 6p	5s ² 5p ³ 6p	5s ² 5p ² 6p	5s ² 5p6p
5s ² 5p ⁶ 6f	5s²5p ⁵ 7p	$5s^25p^47p$	5s²5p³7p	5s²5p²7p	5s²5p7p
5s ² 5p ⁶ 7f	5s ² 5p ⁵ 8p	5s ² 5p ⁴ 8p	5s ² 5p ³ 8p	5s ² 5p ² 8p	5s ² 5p8p
$5s^25p^68f$	$5s^25p^54f$	$5s^25p^44f$	$5s^25p^34f$	$5s^25p^24f$	5s ² 5p4f
$5s^25p^66p$	$5s^25p^55f$	$5s^25p^45f$	$5s^25p^35f$	$5s^25p^25f$	5s ² 5p5f
$5s^{2}5p^{6}7p$	$5s^{2}5p^{5}6f$	$5s^25p^46f$	$5s^2 5p^3 6f$	$5s^25p^26f$	$5s^25p6f$
$5s^25p^68p$	$5s^2 5p^5 7f$	$5s^2 5p^4 7f$	$5s^{2}5p^{3}7f$	$5s^2 5p^2 7f$	$5s^25p7f$
$5s^25p^54f^2$	$5s^2 5p^5 8f$	$5s^25p^48f$	$5s^2 5p^3 8f$	$5s^25p^28f$	$5s^25p8f$
$5s^25p^55d^2$	$5s^25p^44f^2$	$5s^25p^34f^2$	$5s^25p^24f^2$	$5s^25p4f^2$	$5s^24f^2$
$5s^25p^56s^2$	$5s^25p^45d^2$	$5s^25p^35d^2$	$5s^25p^25d^2$	$5s^25p5d^2$	$5s^25d^2$
$5s^25p^55d6s$	$5s^2 5p^4 6s^2$	$5s^2 5p^3 6s^2$	$5s^2 5p^2 6s^2$	$5s^2 5p 6s^2$	$5s^26s^2$
$5s5p^{6}4f5d$	$5s^25p^45d6s$	$5s^25p^35d6s$	$5s^25p^25d6s$	$5s^25p5d6s$	$5s^25d6s$
$5s5p^64f6d$	$5s5p^65d$	$585p^55d$	$5s5p^45d$	$5s5p^35d$	$5s5p^25d$
$5s5p^64f7d$	$5s5p^66d$	$5s5p^{5}6d$	$585p^46d$	$5s5p^36d$	$585p^{2}6d$
$5s5p^{6}4f8d$	$585p^{6}7d$	$585p^{-5}7d$	$585p^{4}7d$	$585p^{-}0d^{-}$	$5s5p^{2}7d$
$5s5p^{6}4f6s$	$5s5p^{6}8d$	$5s5p^{-7}d$ $5s5n^{5}8d$	$5s5p^{4}8d$	$5s5p^{3}8d$	$5s5p^{2}8d$
$5s5p^{6}/f7s$	5.5p ⁶ 6s	585p 64 585p ⁵ 68	5s5p ⁴ 6s	585p 64 585p ³ 68	$5s5p^{2}6s$
585p +178	585p ⁶ 7e	585p 08	5s5p $0s5s5n^{4}7s$	585p ³ 7e	$5s5p^{2}7s$
535P + 103 $5n^{6}/f^{3}$	585p ⁶ 86	585p ⁵ 86	585p ⁴ 86	585p ³ 86	$5s5p^{2}8s$
JP 41	505p51f51	$5_{0}5_{0}4_{1}5_{1}$	505p ³ 1f51	$5_{0}5_{0}^{2}$	5.5p1f51
	585p ⁻ 415d	585p 415d	$585p^{-415d}$	585p 415d $5a5p^24f6d$	585p415u
	585p*410d	585p 410d	585p ⁻ 410d	585p 410d	5s5p4100
	5s5p°417d	585p-41/d	585p°417d	585p-41/d	5s5p417d
	5s5p°418d	5s5p ⁻ 418d	5s5p°418d	5s5p ² 418d	5s5p418d
	5s5p°416s	5s5p+416s	5s5p°416s	$5s5p^2416s$	5s5p4f6s
	5s5p°41/s	5s5p ⁺ 4f/s	5s5p°41/s	5s5p ² 4f/s	5s5p4f/s
	5s5p ³ 4f8s	5s5p ⁴ 4f8s	5s5p°4f8s	5s5p ² 4f8s	5s5p4f8s
	5p ³ 4f ³	$5p^44t^3$	5p ⁰	5p ⁹	5p ⁴
	$5p^{0}4t^{2}$	5p ³ 4f ²	5p44f2	$5p^24t^3$	5p4f ³
		$5p^{\circ}4f$	5p ³ 4f	$5p^{3}4f^{2}$	$5p^24f^2$
				5p ⁴ 4f	5p ³ 4f
Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity
5s ² 5p ⁶ 6s	$5s^25p^56s$	$5s^25p^46s$	5s ² 5p ³ 6s	5s ² 5p ² 6s	5s ² 5p6s
$5s^25p^67s$	$5s^25p^57s$	$5s^25p^47s$	5s ² 5p ³ 7s	$5s^25p^27s$	5s ² 5p7s
$5s^25p^68s$	$5s^25p^58s$	$5s^25p^48s$	5s ² 5p ³ 8s	5s ² 5p ² 8s	5s ² 5p8s
$5s^25p^65d$	$5s^25p^55d$	$5s^25p^45d$	$5s^25p^35d$	$5s^25p^25d$	5s ² 5p5d
$5s^25p^66d$	$5s^25p^56d$	$5s^25p^46d$	$5s^25p^36d$	$5s^25p^26d$	5s ² 5p6d
$5s^25p^67d$	$5s^25p^57d$	$5s^25p^47d$	$5s^25p^37d$	$5s^25p^27d$	5s ² 5p7d
$5s^25p^68d$	$5s^25p^58d$	$5s^25p^48d$	$5s^25p^38d$	$5s^25p^28d$	$5s^25p8d$
$5s^25p^65g$	$5s^{2}5p^{5}5g$	$5s^25p^45g$	$5s^2 5p^3 5g$	$5s^25p^25g$	$5s^25p5g$
$5s^25p^66g$	$5s^25p^56g$	$5s^25p^46g$	$5s^25p^36g$	$5s^25p^26g$	$5s^25p6g$
$5s^25p^67g$	$5s^25p^57g$	$5s^25p^47g$	$5s^2 5p^3 7g$	$5s^25p^27g$	$5s^25p7g$
$5s^25p^68g$	$5s^25p^58g$	$5s^25p^48g$	$5s^25p^38g$	$5s^25p^28g$	5s ² 5p8g
$5s^25p^54f5d$	$5s^25p^44f5d$	$5s^25p^34f5d$	$5s^25p^24f5d$	5s ² 5p4f5d	5s ² 4f5d
$5s^25p^54f6s$	$5s^25p^44f6s$	$5s^25p^34f6s$	$5s^25p^24f6s$	$5s^25p4f6s$	$5s^24f6s$
$5s5p^64f^2$	5s5p ⁶ 6p	5s5p ⁶	5s5p ⁵	$5s5p^4$	$5s5p^3$
5s5p ⁶ 4f6p	$5s5p^67p$	$5s5p^56p$	$5s5p^46p$	$5s5p^36p$	$5s5p^26p$
$5s5p^{6}4f7p$	$5s5p^{6}8p$	$5s5p^57p$	$5s5p^47p$	$5s5p^37p$	$5s5p^27p$
5s5p ⁶ 4f8p	$5s5p^64f$	5s5p ⁵ 8p	$5s5p^48n$	$5s5p^38n$	$5s5p^28n$
$5p^64f^25d$	$5s5p^65f$	$5s5n^54f$	$5s5p^44f$	$5s5n^34f$	$5s5p^24f$
- r	$5s5p^66f$	$5s5p^55f$	$5s5p^45f$	$5s5p^35f$	$5s5p^25f$
	$5s5p^67f$	5s5p ⁵ 6f	$5s5p^46f$	$5s5p^36f$	$5s5p^26f$
	$5s5p^68f$	$5s5p^57f$	$5s5p^47f$	$5s5p^37f$	$5s5p^27f$
	$5s5n^54f^2$	$5s5n^58f$	$5s5p^48f$	$5s5n^{3}8f$	$5s5p^28f$
	$5s5p^{-1}$ $5s5n^{5}4f6n$	$5s5p^{4}4f^{2}$	$5s5p^{-01}$	$5s5p^{-01}$	$5s5p4f^2$
	5s5p = 10p $5s5n^54f7n$	$5_{5}^{5}^{5}^{7}$ -1^{1}	$5s5p^{-41}$ $5s5n^{3}4f6n$	$5_{5}^{5}^{2}$ 5_{5}^{2} 4_{1}^{6} 5_{5}^{6}	5s5p4f6p
	555p = 1/p $555n^54f8n$	$5_{5}^{5}^{5}^{7}$	5s5p = 10p $5s5n^34f7n$	5s5p = 10p $5s5n^24f7n$	5s5p4f7p
	$5n^{5}/f^{2}5d$	5_{5} $p = 1/p$ 5_{5} 5_{n}^{4} 4_{5} p	5s5p ³ /f&p	5_{5} $p = 1/p$ 5_{5} p^{2}/f_{8} p	5s5p4f&p
	$5p^{-41}$ $5u^{-5}$	5n ⁶ 5d	5^{5} 5^{5} 5^{7} 5^{7}	$5^{35}p$ $\pm 10p$ $5n^45d$	$5^{3}5^{4}$
	JP TIJU	Jp Ju	JP Ju	Jp Ju	JP Ju
	•	$5n^4 4f^2 5d$	$5n^44f5d$	$5n^24f^25d$	$5n4f^25d$

Table 3.8: Configurations included in HFR calculations for Pr V–X ions.

In Table 3.9, we summarize the number of levels below the IP and transitions selected for opacity calculations for each Pr ion obtained with HFR approach as well as IPs taken from the NIST database (Kramida et al., 2024).

Table 3.9: Number of levels and lines obtained in HFR calculations for Pr V–X. The ionization potentials are also given for each ion.

Ion	Number of levels ^{<i>a</i>}	Number of lines ^b	$IP (cm^{-1})^c$
Pr V	735	14 534	464 000
Pr VI	3 447	203 360	663 000
Pr VII	7 826	1 017 797	784 000
Pr VIII	7 694	1 028 901	905 000
Pr IX	8 298	1 161 017	1 060 000
Pr X	3 974	865 860	1 195 000

Total number of HFR levels considered in opacity calculations

^b Total number of transitions involving energy levels below the IP with HFR calculated $\log(gf)$ -values ≥ -5

^c Ionization potential taken from NIST (Kramida et al., 2024)

The second method to determine the radiative parameters for those ions, is the MCDHF method (Grant, 2007). In order to compute the atomic structures and radiative parameters in a particular sample of Pr ions, namely Pr V and Pr X the same methodology as the one developed in the previous sections is employed. A set of configurations is used to gradually incorporate valence-valence (VV) and core-valence (CV) correlations for each of these ions. This process creates the multireference (MR), from which all allowed transitions are computed, as shown in Table 3.10.

In the case of Pr V, the MR was chosen to include the $5p^{6}4f$, $5p^{5}4f^{2}$, $5p^{5}5d^{2}$ odd- and $5p^{6}5d$, $5p^{5}4f5d$ even-parity configurations. For this ion, the orbitals 1s to 4f were optimized on the ground configuration (*i.e.* $5p^{6}4f$) while 5d orbital was optimized using the MR configurations, keeping all other orbitals fixed. For Pr X, the MR included the $5s^{2}5p^{2}$, $5s^{2}5p4f$, $5s^{2}4f^{2}$ evenand the $5s5p^{3}$, $5s5p^{2}4f$, $5s^{2}5p5d$ odd-parity configurations. The orbitals 1s to 5p were optimized on the $5s^{2}5p^{2}$ ground configuration while the 4f and 5d orbitals were optimized using the MR configurations, keeping all other orbitals fixed. For both ions, VV1 and VV2 models were built by adding single and double (SD) excitations from 5s, 5p, 5d, 4f to 5s, 5p, 5d, 5f, 5g and to 6s, 6p, 6d, 6f, 5g active orbitals, respectively. Specifically for Pr X, a VV3 was built by enabling the SD excitations to 7s, 7p, 7d, 6f and 5g. From VV2 and VV3 for Pr V and Pr X respectively, a CV model was then built. Concerning Pr V, SD excitations were added from the 4d core orbital to the MR valence orbitals, namely 5s, 5p, 5d, and 4f, while for Pr X they were added to VV1. This gave rise to a total of 667 030 and 767 797 configuration state functions (CSFs), for the odd- and even-parities, for Pr V and 215 456 and 623 974 CSFs in the odd- and even-parities of Pr X as it is summarized in Table 3.10.

For Pr V and Pr X, a comparison of our MCDHF energy level values obtained in CV models showed a good agreement with the experimental data reported in the literature (Kaufman and Sugar (1967) for Pr V and Bekker et al. (2019) for Pr X), the mean deviation $\Delta E/E_{exp}$ (with $\Delta E = E_{MCDHF} - E_{exp}$) being found to be equal to 0.018 ± 0.09 (Pr V) and 0.126 ± 0.09 (Pr X).

Calculation	Pr V	Pr X
MR	Odd parity	Even parity
	$5p^64f$	$5s^25p^2$
	$5p^54f^2$	$5s^25p4f$
	$5p^55d^2$	$5s^24f^2$
	Even parity	Odd parity
	$5n^65d$	5s5n ³
	$5p^{5}4f5d$	$5s5p^24f$
	- I	$5s^25p5d$
		1
VV1	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}
VV2	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}
VV3		{7s,7p,7d,6f,5g}
CV	{5s,5p,5d,4f}	{5s,5p,5d,5f,5g}
CSFs	1 434 827	839 430

Table 3.10: Computational strategies used in MCDHF calculations for Pr V and Pr X ions.

Lastly, in a third computational step, the level energies and radiative parameters of these two lanthanide ions, *i.e.* Pr V and Pr X, were determined using the configuration interaction and many-body perturbation-theory (CI+MBPT) method as implemented in the AMBiT atomic structure code by Kahl and Berengut (2019). More particularly, the AMBiT program's emu CI approximation (Geddes et al., 2018) was used in Pr V in order to minimize the problem's size without sacrificing much accuracy.

The AMBiT calculations were focused on the properties of the experimental energy levels found in the literature. As previously cited in the beginning of this section, there are 8 levels belonging to the configurations 4f, 5d, 6s, 6p and 7s determined by Kaufman and Sugar (1967) for Pr V and 15 levels of Pr X belonging to the even configurations $5s^25p^2$ and $5s^25p4f$ published by Bekker et al. (2019). For all the AMBiT calculations, QED and Breit interactions were included.

In Pr V, the core spin-orbitals and the frozen core potential were generated by solving the Dirac–Hartree–Fock (DHF) equations for the Xe-like ground configurations [Pd]5s²5p⁶ consisting in 54 electrons. The valence orbitals were determined by diagonalizing a set of *B*-splines using the DHF hamiltonian with the frozen core potential. The emu CI expansions with symmetries as $J^{\pi} = 1/2^{\text{even}}-5/2^{\text{even}}$, $1/2^{\text{odd}}-7/2^{\text{odd}}$ were obtained by considering, for the large side, the SD electron and hole excitations from leading configurations 4f, 6p, 5d, 6s and 7s to the active set of orbitals {15s, 15p, 15d, 15f, 15g, 15h} with all the core orbitals lower than 5s inactive, *i.e.* 5s to 15s, 5p to 15p, 5d to 15d, 4f to 15f, 5g to 15g and 6h to 15h. For the small side, the active set of orbitals was reduced to {8s, 8p, 8d, 8f, 8g, 8h} when considering double electron excitations and only single hole excitations. The resulting emu CI matrix dimensions were N = 9 720 262 for the large side and $N_{\text{small}} = 64$ 101 for the small side. One, two and three body MBPT diagrams (Berengut and Flambaum, 2006) involving the frozen core orbitals and virtual orbitals up to {30s, 30p, 30d, 30f, 30g, 30h} were considered in the evaluation of the operator matrix elements. The relative differences, $\Delta E = (E_{\text{cal}} - E_{\text{exp}})/E_{\text{exp}}$, with respect to the experimental

energy levels published by Kaufman and Sugar (1967) ranged from more than 1% to 3% with an average of 2.2% and a standard deviation of 0.6%.

Concerning Pr X, the DHF equations were solved in a first step for the ground configuration of the Pd-like Pr XIV system, *i.e.* [Kr]4d¹⁰, with 46 electrons in order to obtain the core orbitals. This enabled us to build in a second step the core electron potential and to solve the frozen core DHF equations for the valence orbitals. In the CI step, the 50-electron wavefunction expansions with symmetries as $J^{\pi} = 0^{\text{even}} - 12^{\text{even}}$, $0^{\text{odd}} - 11^{\text{odd}}$ were generated by considering all the single electron excitations from the $5s^25p^2$, $5s^24f^2$, $5s^25p4f$, $5s5p^3$, $5s5p^24f$, $5s5p4f^2$, $5s4f^3$, $5p^4$, $4f^4$, $5p^34f$, $5p4f^3$ and $5p^24f^2$ leading configurations to the {6s, 6p, 6d, 5f} active set keeping all the core orbitals lower than 5s inactive. The dimension of the CI matrix was N = 8 561. In the MBPT step, one, two and three body diagrams were considered involving the frozen core orbitals and virtual orbitals belonging to the set {30s, 30p, 30d, 30f, 30g, 30h}. The relative differences, $\Delta E/E_{\text{exp}}$, between our eigenvalues and the available experimental energy levels (Bekker et al., 2019) ranged from -3.4% to 1.3% with an average of -1.3% and a standard deviation of 1.2%.

As mentioned for La and Ce ions, HFR method gives the greatest number of transitions since we can include much more spectroscopic configurations in this approach (see Table 3.9). Therefore, the MCDHF and AMBiT results are important to benchmark the HFR results performed in the selected ions. The HFR transition probabilities and oscillator strengths calculated in this work are listed for all the experimentally observed lines published so far for the Pr ions of interest in Table C.1 in Appendix C. The latter where experimentally lines are reported from Kaufman and Sugar (1967) only concern Pr V.

For very few transitions, other oscillator strengths were also published for Pr V. They agree well (usually within a few percent) with our values. For instance, we found average deviations between our HFR gf-values and previous theoretical data of 9%, 8%, 8%, 14% and 6% when comparing with the relativistic single-configuration Hartree-Fock calculations of Migdalek and Baylis (1979), the relativistic model potential approach of Migdalek and Wyrozumska (1987), the relativistic many-body perturbation calculations of Savukov et al. (2003), the Dirac-Fock computations of Zilitis (2014), and the relativistic Hartree-Fock calculations of Karacoban and Dogan (2015), respectively. The log(gf)-values deduced from all these previous works are compared to those obtained in the present work in Table C.1.

More intriguing are the cross-tabulations that we performed for a few chosen ions between our HFR, MCDHF, and AMBiT computations. Such comparisons are illustrated in Figures 3.9 and 3.10 where the HFR oscillator strengths are plotted as function of the results obtained with the two other methods. More precisely, in Figure 3.9, the HFR $\log(gf)$ -values are compared with those computed using the MCDHF method for transitions involving the ground levels in Pr V and Pr X while in Figure 3.10, the same type of comparison is made with the data obtained using emu CI and CI+MBPT approach (AMBiT) for Pr V and Pr X, respectively. In those cases, we noted an overall good agreement, the average relative differences between HFR and MCDHF oscillator strengths being found to be within 15% whereas the mean deviations between HFR and AMBiT gf-values were found to be within 25%. But for some particular transitions, greater differences between the three approaches were noted. These were primarily due to computed line strengths that were strongly impacted by cancellation effects. Nevertheless, these comparisons indicate that we can suppose oscillator strengths determined in our work to be affected by

uncertainties of the order of 30% for the strongest lines $(\log(gf) \ge -1)$ and a factor of two for weaker lines.



Figure 3.9: Comparison between the oscillator strengths (log(gf)) computed in this work using HFR and MCDHF methods for lines involving the ground level in Pr V and Pr X ions.



Figure 3.10: Comparison between the oscillator strengths (log(gf)) computed in this work using HFR and emu CI (Pr V) and CI+MBPT (Pr X) (AMBiT) methods for lines involving the ground level for both ions.

3.1.4 Nd V–X ions

Among the studies published for Nd ions, Meftah et al. (2008) identified 160 lines of Nd V using vacuum ultraviolet normal incidence spectroscopy of a sliding spark source between 710 – 2 240 Å. The analysis of this spectrum allowed to determine 48 energy levels belonging to the $5p^{6}4f^{2}$, $5p^{6}4f5d$, $5p^{6}4f6s$ and $5p^{6}4f6p$ configurations. Delghiche et al. (2015), then, extended the Nd V spectrum observation in the laboratory to a shorter wavelength region, down to 370 Å. This investigation resulted in the determination of 104 energy levels of the $5p^{5}4f^{2}5d$ core-excited configuration.

As for Pr ions, a few radiative parameter calculations were published theoretically for a restricted set of electric dipole transitions. Concerning Nd V, the largest radiative data set was published by Meftah et al. (2008) and Delghiche et al. (2015) who implemented the HFR method to compute the transition probabilities for all the lines they observed in the laboratory. The present study is a major extension of Stanek and Migdalek (2004) earlier work, which reported multiconfiguration Dirac-Fock oscillator strengths for only the Nd V 6s² ¹S₀ – 6s6p ^{1,3}P₁ transitions. Such as for Pr ions, some other studies about oscillator strength calculations were published, on the one hand, by Glushkov (1992) and Zilitis (2014) using the relativistic model potential and the Dirac-Fock method, respectively, for some resonance transitions involving low-lying configurations along the Cs isoelectronic sequence, including Nd VI, and on the other hand, those carried out by Cheng and Froese Fischer (1983) using term-dependent Hartree-Fock technique for the 4d¹⁰ – 4d⁹nf ¹P transitions in Xe-like ions, including Nd VII.

The same methodology was employed, as in the three previous sections, to compute the atomic structure. We first computed the electronic structure using HFR procedure (Cowan, 1981). For each ion, the HFR physical model retained was based, as for La, Ce and Pr ions, on a Pd-like ionic core with 46 electrons filling all the subshells up to $4d^{10}$ surrounded by k valence electrons, with k ranging from 5 to 10, depending on the total number of electrons in the atomic system. Table 3.11 summarizes the large number of interacting configurations introduced in this method.

Among the six ions considered in this section, only one has experimentally measured wavelengths for electric dipole transitions, namely Nd V (Meftah et al., 2008; Delghiche et al., 2015), as mentioned before. When comparing our HFR values with these experimental data, we found an overall good agreement (smaller than 2% in most cases), the average differences $\Delta \lambda / \lambda_{Obs}$ (with $\Delta \lambda = \lambda_{HFR} - \lambda_{Obs}$) being found to be equal to -0.012 ± 0.049 .

In Table 3.12, we give an overview of the number of levels calculated below the IP taken from the NIST database (Kramida et al., 2024) and the number of transitions for these Nd ions.

Nd V	Nd VI	Nd VII	Nd VIII	Nd IX	Nd X
Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity
$5s^25p^64f^2$	$5s^25p^64f$	$5s^25p^6$	$5s^25p^5$	5s ² 5p ³ 4f	$5s^25p^24f$
5s ² 5p ⁶ 4f5f	5s ² 5p ⁶ 5f	5s ² 5p ⁵ 6p	5s ² 5p ⁴ 6p	5s ² 5p ³ 5f	5s ² 5p ² 5f
5s ² 5p ⁶ 4f6f	$5s^25p^66f$	$5s^25p^57p$	$5s^25p^47p$	5s ² 5p ³ 6f	$5s^25p^26f$
5s ² 5p ⁶ 4f7f	5s ² 5p ⁶ 7f	5s ² 5p ⁵ 8p	5s ² 5p ⁴ 8p	5s ² 5p ³ 7f	$5s^25p^27f$
$5s^25p^64f8f$	$5s^25p^68f$	$5s^25p^54f$	$5s^25p^44f$	$5s^25p^38f$	$5s^25p^28f$
5s ² 5p ⁶ 4f6p	5s ² 5p ⁶ 6p	5s ² 5p ⁵ 5f	$5s^25p^45f$	$5s^25p^4$	$5s^25p^3$
5s ² 5p ⁶ 4f7p	5s ² 5p ⁶ 7p	5s ² 5p ⁵ 6f	$5s^25p^46f$	5s ² 5p ³ 6p	5s ² 5p ² 6p
5s ² 5p ⁶ 4f8p	5s ² 5p ⁶ 8p	$5s^25p^57f$	$5s^25p^47f$	5s ² 5p ³ 7p	5s ² 5p ² 7p
$5s^25p^65d^2$	$5s^25p^54f^2$	$5s^25p^58f$	$5s^25p^48f$	5s ² 5p ³ 8p	5s ² 5p ² 8p
5s ² 5p ⁶ 5d6d	$5s^25p^55d^2$	$5s^25p^44f^2$	$5s^25p^34f^2$	$5s^25p^24f^2$	5s ² 5p4f ²
$5s^25p^65d7d$	$5s^25p^56s^2$	$5s^25p^45d^2$	$5s^25p^35d^2$	$5s^25p^25d^2$	5s ² 5p5d ²
$5s^25p^65d8d$	$5s^25p^55d6s$	$5s^25p^46s^2$	$5s^25p^36s^2$	$5s^25p^26s^2$	5s ² 5p6s ²
5s ² 5p ⁶ 6s ²	5s5p ⁶ 4f5d	$5s^25p^45d6s$	$5s^25p^35d6s$	$5s^25p^25d6s$	5s ² 5p5d6s
5s ² 5p ⁶ 5d6s	5s5p ⁶ 4f6d	5s5p ⁶ 5d	5s5p ⁵ 5d	5s5p ⁴ 5d	5s5p ³ 5d
5s ² 5p ⁶ 5d7s	5s5p°4f7d	5s5p°6d	5s5p ^o 6d	5s5p ⁴ 6d	5s5p ³ 6d
5s ² 5p ⁰ 5d8s	5s5p ⁶ 4f8d	5s5p ⁶ 7d	5s5p ⁵ 7d	5s5p ⁴ 7d	5s5p ³ 7d
$5s5p^{\circ}4f^{2}5d$	5s5p ⁶ 4f6s	5s5p°8d	5s5p ⁹ 8d	5s5p ⁴ 8d	5s5p ³ 8d
$5s5p^{6}4f^{2}6d$	5s5p ⁶ 4f7s	5s5p°6s	5s5p ⁵ 6s	$5s5p^46s$	5s5p°6s
$5s5p^{6}4f^{2}7d$	5s5p°4f8s	5s5p ⁶ 7s	$5s5p^{5}7s$	$5s5p^47s$	5s5p°7s
$5s5p^{\circ}4f^{2}8d$	$5p^{0}4f^{3}$	5s5p°8s	5s5p ⁹ 8s	5s5p ⁴ 8s	5s5p ³ 8s
$5s5p^{6}4f^{2}6s$		5s5p ³ 4f5d	5s5p ⁴ 4f5d	5s5p ³ 4f5d	5s5p ² 4f5d
$5s5p^{6}4f^{2}/s$		5s5p ⁹ 4f6d	5s5p ⁺ 4f6d	$5s5p^{3}4f6d$	$5s5p^24f6d$
$5s5p^{\circ}4f^{2}8s$		$5s5p^{9}4f/d$	$5s5p^{4}4f/d$	$5s5p^{3}4f/d$	$5s5p^24f/d$
5s ² 5p ⁶ 4f ⁶		5s5p°418d	5s5p*418d	5s5p°4f8d	5s5p ² 4f8d
		5s5p°416s	$5s5p^{-}416s$	$5s5p^{\circ}416s$	$5s5p^{-}410s$
		5s5p°417s	$5s5p^{-}41/s$	$5s5p^{\circ}41/s$	$5s5p^{-41}/s$
		5s5p*418s	$5s_{2}p^{-41}$	555p°4185	5s5p-418s
		$5p^{6}4f^{2}$	$5p^{41^{2}}$	$5p^4$	$5p^{2}4f^{3}$
		5p 4i	$5p^{6}4f$	5p 41 $5p^54f$	$5p^{-41}$ $5n^{3}4f^{2}$
			5p 4i	3p 4i	$5p^{41}$ $5p^{4}4f$
0.11	F '(F	0.11	Sp 41
Odd parity $5a^25m^6466a$	Even parity $5a^25a^66a$	Odd parity $5a^25\pi^56a$	Even parity $5a^25\pi^46a$	Odd parity $5a^25a^36a$	Even parity $5a^25\pi^26a$
$5s^{-}5p^{\circ}410s$ $5s^{2}5p^{6}4f7s$	$5s^{2}5p^{6}7c$	$5s^{2}5p^{5}0s$	$5s^{2}5p^{2}0s$	$5s^{2}5p^{3}0s$	$5s^{2}5p^{2}7c$
$5s^{2}5p^{6}4f^{8}s$	$5s^{2}5p^{6}8s$	$5s^{2}5p^{5}8s$	5s 3p 7s $5s^25p^48s$	$5s^{2}5n^{3}8c$	$5s^{2}5p^{2}8s$
$5s^{2}5p^{6}4f5d$	5s 5p 6s $5s^2 5p^6 5d$	$5s^{2}5p^{5}5d$	5s 5p 8s $5s^25p^45d$	5s 5p 8s $5s^2 5p^3 5d$	$5s^{2}5p^{2}5d$
$5s^{2}5p^{6}4f6d$	$5s^{2}5p^{6}6d$	$5^{\circ}{}^{5}{}^{5}{}^{5}{}^{6}{}^{d}$	$5^{8} 5^{2} 5^{4} 6d$	$5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 6^{\circ} 4$	$5s^{2}5p^{2}6d$
$5s^25p^64f7d$	$5s^{2}5p^{6}7d$	$5s^{2}5p^{5}7d$	$5s^{2}5p^{4}7d$	$5s^{2}5p^{3}7d$	$5s^{2}5p^{2}7d$
$5s^25p^64f8d$	$5s^25p^68d$	$5s^25p^58d$	$5s^25p^48d$	$5s^25p^38d$	$5s^25p^28d$
$5s^25p^64f5g$	$58^{2}5p^{6}5q$	$5s^25p^55g$	$5s^25p^45q$	$5s^25n^35g$	$5s^25p^25q$
$5s^25p^64f6g$	$5s^25p^66g$	$5s^25p^56g$	$5s^25p^46g$	$5s^25p^36g$	$5s^25p^26g$
$5s^25p^64f7g$	$5s^25p^67g$	$5s^25p^57g$	$5s^25p^47g$	$5s^25p^37g$	$5s^25p^27g$
$5s^25p^64f8g$	$5s^25p^68g$	$5s^25p^58g$	$5s^25p^48g$	$5s^25p^38g$	$5s^25p^28g$
$5s^25p^65d6p$	$5s^25p^54f5d$	$5s^25p^44f5d$	$5s^25p^34f5d$	$5s^25p^24f5d$	$5s^25p4f5d$
$5s^25p^65d7p$	$5s^25p^54f6s$	$5s^25p^44f6s$	5s ² 5p ³ 4f6s	$5s^25p^24f6s$	5s ² 5p4f6s
$5s^25p^65d8p$	$5s5p^{6}4f^{2}$	5s5p ⁶ 6p	$5s5p^{6}$	$5s5p^{5}$	$5s5p^4$
$5s^25p^65d5f$	5s5p ⁶ 4f6p	5s5p ⁶ 7p	5s5p ⁵ 6p	5s5p ⁴ 6p	5s5p ³ 6p
$5s^25p^65d6f$	5s5p ⁶ 4f7p	5s5p ⁶ 8p	5s5p ⁵ 7p	$5s5p^47p$	$5s5p^37p$
5s ² 5p ⁶ 5d7f	5s5p ⁶ 4f8p	5s5p ⁶ 4f	5s5p ⁵ 8p	5s5p ⁴ 8p	5s5p ³ 8p
$5s^25p^65d8f$	$5p^64f^25d$	5s5p ⁶ 5f	5s5p ⁵ 4f	5s5p ⁴ 4f	5s5p ³ 4f
$5s^25p^54f^25d$		5s5p ⁶ 6f	5s5p ⁵ 5f	5s5p ⁴ 5f	5s5p ³ 5f
$5s^25p^54f^26s$		5s5p ⁶ 7f	5s5p ⁵ 6f	5s5p ⁴ 6f	5s5p ³ 6f
$5s^25p^55d^3$		5s5p ⁶ 8f	$5s5p^{5}_{-}7f$	5s5p ⁴ 7f	$5s5p^37f$
$5s5p^64f^3$		$5s5p^54f^2$	5s5p ⁵ 8f	5s5p ⁴ 8f	5s5p ³ 8f
5s5p ⁶ 4f ² 6p		5s5p ⁵ 4f6p	$5s5p^44f^2$	5s5p ³ 4f ²	$5s5p^24f^2$
$5s5p^64f^27p$		5s5p ⁵ 4f7p	5s5p ⁴ 4f6p	5s5p ³ 4f6p	5s5p ² 4f6p
5s5p ⁶ 4f ² 8p		5s5p ⁵ 4f8p	5s5p ⁴ 4f7p	5s5p ³ 4f7p	5s5p ² 4f7p
		$5p^{5}4f^{2}5d$	5s5p ⁴ 4f8p	5s5p ³ 4f8p	5s5p ² 4f8p
		5p°4f5d	5p°5d	5p°5d	$5p^45d$
			5p*4t25d	5p*415d	$5p^24t^25d$
			5p°4f5d		5p°4f5d

Table 3.11: Configurations included in HFR calculations for Nd V–X ions.

Ion	Number of levels ^{<i>a</i>}	Number of lines ^b	$IP (cm^{-1})^c$
Nd V	2 164	211 796	483 900
Nd VI	735	22 151	676 000
Nd VII	3 447	497 534	799 000
Nd VIII	7 826	1 122 652	923 000
Nd IX	7 694	1 101 470	1 093 000
Nd X	8 298	1 159 387	1 224 000

Table 3.12: Number of levels and transitions obtained in HFR calculations for Nd V–X. The ionization potentials are also given for each ion.

^a Total number of HFR levels considered in opacity calculations

^b Total number of transitions involving energy levels below the IP with HFR calculated $\log(gf)$ -values ≥ -5

^c Ionization potential taken from NIST (Kramida et al., 2024)

As for the three lanthanides presented before, namely La, Ce and Pr, the MCDHF approach was the second method used to obtain atomic data for Nd V and Nd VI. A summary of the configuration list that was included to gradually incorporate valence-valence (VV) and core-valence (CV) correlations for each of these two ions is shown in Table 3.13.

For Nd V, the MR consisted of $5p^64f^2$, $5p^65d^2$ even- and $5p^64f5d$, $5p^55d^3$ odd-parity configurations. In the case of Nd VI, the MR was chosen to include the $5p^64f$, $5p^54f^2$, $5p^55d^2$ oddand $5p^65d$, $5p^54f5d$ even-parity configurations. For these ions, orbitals 1s to 4f were optimized on the respective ground configurations (*i.e.* $5p^64f^2$ for Nd V and $5p^64f$ for Nd VI) while 5d orbital was optimized using the MR configurations, keeping all other orbitals fixed. VV1 and VV2 models were built by adding SD excitations from 5s, 5p, 5d, 4f to 5s, 5p, 5d, 5f, 5g and to 6s, 6p, 6d, 6f, 5g active orbitals, respectively. From the latter, a CV model was then built by adding SD excitations from the 4d core orbital to the MR valence orbitals, namely 5s, 5p, 5d, and 4f. For Nd VI, this gave rise to a total of 667 030 and 767 797 configuration state functions (CSFs), for the odd- and even-parities, respectively and for Nd V to 142 859 and 842 073 CSFs, for the even- and odd-parities, respectively.

For Nd V, a comparison of our MCDHF energy level values obtained in CV models showed a good agreement with the experimental data reported in the literature (Meftah et al., 2008; Delghiche et al., 2015), the mean deviation $\Delta E/E_{exp}$ (with $\Delta E = E_{MCDHF} - E_{exp}$) being found to be equal to 0.006 \pm 0.063.

Calculation	Nd V	Nd VI
MR	Even parity	Odd parity
	$5p^64f^2$	5p ⁶ 4f
	$5p^65d^2$	$5p^54f^2$
		$5p^55d^2$
	Odd nority	Evon pority
	5 n ⁶ 4 f 5 d	Even parity
	5p ⁻ 4130	5p ⁻ 5d 5p ⁵ 4f5d
	Sp [*] Su [*]	5p*415u
VV1	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}
VV2	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}
CV	{5s,5p,5d,4f}	{5s,5p,5d,4f}
CSFs	984 932	1 434 827

Table 3.13: Computational strategies used in MCDHF calculations for Nd V and Nd VI ions.

Finally, the CI+MBPT method was the third method used to compute the level energies and radiative parameters of Nd V using the AMBiT package (Kahl and Berengut, 2019). Those calculations were focused on the properties of the experimental energy levels found in the literature, *i.e.* for Nd V, 152 levels reported by Meftah et al. (2008) and Delghiche et al. (2015) and belonging to the configurations $5s^25p^64f^2$, $5s^25p^64f5d$, $5s^25p^64f6s$, $5s^25p^64f6p$ and $5s^25p^54f^25d$. For all the AMBiT calculations, QED and Breit interactions were included.

In Nd V, the frozen core potential and the corresponding orbitals were determined by solving the DHF equations for the ground configuration of the Xe-like Nd VII, *i.e.* [Kr]4d¹⁰5s²5p⁶. These were then applied to obtain the valence orbitals and solve the frozen-core DHF equations for the 56-electron Nd V atomic system. The CI matrix is then built by considering a set of interacting configurations with symmetries $J^{\pi} = 0^{\text{even}}-6^{\text{even}}$, $0^{\text{odd}}-5^{\text{odd}}$ generated by SD electron and hole excitations to the {6s, 6p, 6d, 6f, 6g} active set of orbitals from the leading configurations 4f² and 4f5d keeping inactive the orbitals of the Pd-like Nd XV frozen core, *i.e.* from 1s up to 4d. The dimension of the CI matrix was N = 1 708 459. Finally, the one, two, and three body diagrams involving the Pd-like frozen core orbitals and virtual orbitals up to {30s, 30p, 30d, 30f, 30g, 30h} were evaluated in order to add the MBPT corrections to the projected effective multielectron Hamiltonian matrix. The relative differences with the experimental level energies of Meftah et al. (2008); Delghiche et al. (2015) ranged from -2% to 11% with an average of 6.7% and a standard deviation of 3.5%.

Among the three theoretical methods, HFR gave the greatest number of transitions compared to the CI+MBPT and MCDHF approaches, serving thus as benchmarking methods. Therefore, the HFR transition probabilities and oscillator strengths obtained in the present work are listed for all the experimentally observed lines published by Meftah et al. (2008); Delghiche et al. (2015) for Nd V in Table D.1 in Appendix D. In the latter, gA-values obtained by Meftah et al. (2008); Delghiche et al. (2008); Delghiche et al. (2015) who used HFR method but with much more limited bases of interacting configurations than the one considered in our work are also given. The agreement between the two sets of results reflects this, and although it is generally satisfactory, there are some notable

deviations for several transitions.

We also compared, as for the previous elements, results between our HFR, MCDHF and CI+MBPT calculations. Such comparisons (log(gf)-values) are illustrated in Figures 3.11 and 3.12 where the HFR oscillator strengths are plotted as a function of the results obtained with the two other methods. More precisely, in Figure 3.11, the HFR log(gf)-values are compared with those computed using the MCDHF method for transitions involving the ground level in Nd V and Nd VI ions, while in Figure 3.12, the same type of comparison is made with the data obtained using the CI+MBPT results (AMBiT) for the Nd V ion. In the overall, we observed a good agreement in these cases: mean deviations between HFR and CI+MBPT (AMBiT) gf-values were found to be within 35%, while the average relative differences between HFR and MCDHF oscillator strengths were found to be within 10%. However, as for Pr ions, some discrepancies between the three methods can be observed for some specific transitions mostly characterized by computed line strengths affected by strong cancellation effects (CF < 0.05) or by large disagreements between length (Babushkin) and velocity (Coulomb) gauge formalisms (30%).



Figure 3.11: Comparison between the oscillator strengths (log(gf)) computed in this work using HFR and MCDHF methods for lines involving the ground level in Nd V and Nd VI ions.



Figure 3.12: Comparison between the oscillator strengths (log(gf)) computed in this work using HFR and CI+MBPT (AMBiT) methods for lines involving the ground level in Nd V.

3.1.5 Pm V–X ions

Concerning Pm ions, there is no experimental data published to date to our knowledge. It is thus challenging to determine the right potential to use in order to obtain orbitals representing the ion in the CI+MBPT approach. Therefore, we only calculate atomic data with HFR and MCDHF methods and compared those theoretical results between them. As previously done, we started by calculating the atomic structure for the sample of Pm ions using HFR (Cowan, 1981). For each ion, the HFR physical model used was based, as for the aforementioned ions, on a Pd-like ionic core with 46 electrons with all the subshells filled up to $4d^{10}$ surrounded by k valence electrons, with k ranging from 6 to 11, depending on the total number of electrons in the atomic system. Table 3.14 summarizes the large number of interacting configurations introduced in this approach.

Pm V	Pm VI	Pm VII	Pm VIII	Pm IX	Pm X
Odd parity	Even parity	Odd parity	Even parity	Odd parity	Even parity
$5s^25p^64f^3$	$5s^25p^64f^2$	$5s^25p^64f$	$5s^25p^44f^2$	$5s^25p^34f^2$	$5s^25p^24f^2$
$5s^25p^64f^25f$	5s ² 5p ⁶ 4f5f	5s ² 5p ⁶ 5f	$5s^25p^54f$	$5s^25p^35d^2$	$5s^25p^25d^2$
$5s^25p^64f^26f$	5s ² 5p ⁶ 4f6f	5s ² 5p ⁶ 6f	$5s^25p^55f$	$5s^25p^36s^2$	$5s^25p^26s^2$
5s ² 5p ⁶ 4f ² 7f	5s ² 5p ⁶ 4f7f	5s ² 5p ⁶ 7f	$5s^25p^56f$	$5s^25p^5$	$5s^25p^34f$
$5s^25p^64t^28t$	$5s^25p^64t8t$	$5s^25p^68t$	$5s^{2}5p^{3}/f$	5s ² 5p ⁴ 6p	$5s^25p^35t$
$5s^2 5p^6 4f^2 6p$ $5s^2 5n^6 4f^2 7n$	$5s^2 5p^6 4f 6p$	$5s^2 5p^6 6p$	$5s^2 5p^6 81$	$5s^{2}5p^{4}/p$	$5s^2 5p^3 6f$
5s 3p 41 7p $5s^2 5n^6 4f^2 8n$	5s 5p 417p $5s^2 5n^6 4f 8n$	58 5p 7p $58^{2}5n^{6}8n$	58.5p $58^{2}5n^{5}6n$	$5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 4^{\circ} 4^{\circ} f$	58 5p 71 58^25n^38f
$5s5p^{6}4f^{3}5d$	$5s^{2}5n^{6}5d^{2}$	$5s^{2}5p^{5}4f^{2}$	$5s^{2}5p^{5}7p$	$5s^{2}5p^{4}5f$	$5s^{2}5p^{4}$
$5s5p^{6}4f^{3}6d$	$5s^25p^65d6d$	$5s^25p^55d^2$	$5s^25p^58p$	$5s^{2}5p^{4}6f$	$5s^25p^36p$
$5s5p^64f^37d$	$5s^25p^65d7d$	$5s^25p^56s^2$	$5s^25p^45d^2$	$5s^25p^47f$	$5s^25p^37p$
$5s5p^64f^38d$	$5s^25p^65d8d$	$5s^25p^55d6s$	$5s^25p^46s^2$	$5s^25p^48f$	$5s^25p^38p$
$5s5p^64f^36s$	$5s^25p^66s^2$	5s5p ⁶ 4f5d	$5s^25p^45d6s$	$5s^25p^35d6s$	$5s^25p^25d6s$
$5s5p^64f^37s$	$5s^25p^65d6s$	5s5p ⁶ 4f6d	5s5p ⁶ 5d	$5s5p^55d$	5s5p ⁴ 5d
$5s5p^{6}4f^{3}8s$	$5s^25p^65d7s$	5s5p ⁶ 4f7d	5s5p ⁶ 6d	5s5p ⁵ 6d	5s5p ⁴ 6d
5s ² 5p ⁶ 5d ² 6p	$5s^{2}5p^{0}5d8s$	5s5p ⁶ 4f8d	5s5p ⁶ 7d	$5s5p^{3}7d$	5s5p ⁴ 7d
$5s^25p^05d^2/p$	$5s5p^{6}4f^{2}5d$	5s5p ⁶ 4f6s	5s5p ⁶ 8d	5s5p ⁹ 8d	5s5p ⁴ 8d
$5s^{2}5p^{6}5d^{2}5f$	$5s5p^{6}4f^{2}7d$	$5s5p^{\circ}41/s$ $5s5p^{6}4f8s$	$5s5p^{\circ}0s$	$5s5p^{\circ}6s$ $5s5p^{5}7s$	$5s5p^{2}os$ $5s5p^{4}7s$
$5s^25n^65d^26f$	$5s5p^{-41}/d$ $5s5n^{6}4f^{2}8d$	550p + 108 $5n^{6}4f^{3}$	5s5p ⁶ 8s	5s5p ⁵ 8s	5s5p ⁴ 8s
$5s^25p^65d^27f$	$5s5p^{6}4f^{2}6s$	50 41	$5s5p^{5}4f5d$	$5s5p^{4}4f5d$	$5s5p^{3}4f5d$
$5s^25p^65d^28f$	$5s5p^{6}4f^{2}7s$		5s5p ⁵ 4f6d	5s5p ⁴ 4f6d	$5s5p^34f6d$
I	$5s5p^64f^28s$		5s5p ⁵ 4f7d	$5s5p^44f7d$	5s5p ³ 4f7d
	$5s^2 \hat{5}p^5 4f^3$		5s5p ⁵ 4f8d	5s5p ⁴ 4f8d	5s5p ³ 4f8d
			5s5p ⁵ 4f6s	5s5p ⁴ 4f6s	5s5p ³ 4f6s
			5s5p ⁵ 4f7s	5s5p ⁴ 4f7s	5s5p ³ 4f7s
			5s5p ⁵ 4f8s	5s5p ⁴ 4f8s	$5s5p^34f8s$
			$5p^{5}4f^{3}$	$5p^44f^3$	$5p^{\circ}$
			5p°412	$5p^{6}4f^{2}$	$5p^{4}1^{2}$
Even parity	Odd parity	Even parity	Odd parity	Sp 41 Even parity	Odd parity
$5s^25n^65d^3$	$5s^25n^64f6s$	$5s^25n^66s$	$5s^25n^56s$	$5s^25n^46s$	$5s^25n^36s$
$5s^25p^65d^26d$	$5s^25p^64f7s$	$5s^{2}5p^{6}7s$	$5s^25p^57s$	$5s^25p^47s$	$5s^25p^37s$
$5s^25p^65d^27d$	$5s^25p^64f8s$	$5s^25p^68s$	$5s^25p^58s$	$5s^25p^48s$	$5s^25p^38s$
$5s^25p^65d^28d$	$5s^25p^64f5d$	$5s^25p^65d$	$5s^25p^55d$	$5s^25p^45d$	$5s^25p^35d$
$5s^25p^65d^26s$	5s ² 5p ⁶ 4f6d	$5s^25p^66d$	$5s^25p^56d$	$5s^25p^46d$	$5s^25p^36d$
$5s^25p^65d^27s$	5s ² 5p ⁶ 4f7d	$5s^25p^67d$	$5s^25p^57d$	$5s^25p^47d$	$5s^25p^37d$
$5s^25p^65d^28s$	5s ² 5p ⁶ 4f8d	$5s^25p^68d$	$5s^25p^58d$	$5s^25p^48d$	$5s^25p^38d$
$5s^25p^64f^26s$	5s ² 5p ⁶ 4f5g	5s ² 5p ⁶ 5g	$5s^25p^55g$	5s ² 5p ⁴ 5g	5s ² 5p ³ 5g
$5s^2 5p^6 4t^2 / s$	$5s^25p^64t6g$	$5s^25p^66g$	$5s^25p^36g$	$5s^25p^46g$	$5s^25p^36g$
$5s^{-}5p^{*}41^{-}8s$ $5s^{2}5p^{6}4f^{2}5d$	$5s^{-}5p^{*}41/g$ $5s^{2}5p^{6}4f8g$	$3s^{-}3p^{\circ}/g$	$3s^{-}3p^{*}/g$	$5s^{2}5p^{4}8a$	$5s^{2}5p^{3}8a$
$5s^{2}5p^{6}4f^{2}6d$	$5s^{2}5n^{6}5d6n$	$5s^{2}5p^{5}4f5d$	$5s^{2}5p^{4}4f5d$	$5s^{2}5p^{3}4f5d$	$5s^{2}5p^{2}4f5d$
$5s^{2}5p^{6}4f^{2}7d$	$5s^{2}5p^{6}5d7p$	$5s^{2}5p^{5}4f6s$	$5s^{2}5p^{4}4f6s$	$5s^{2}5p^{3}4f6s$	$5s^25p^24f6s$
$5s^25p^64f^28d$	$5s^25p^65d8p$	$5s5p^64f^2$	5s5p ⁶ 6p	$5s5p^6$	$5s5p^5$
$5s^25p^64f^25g$	$5s^25p^65d5f$	5s5p ⁶ 4f6p	5s5p ⁶ 7p	5s5p ⁵ 6p	5s5p ⁴ 6p
$5s^25p^64f^26g$	5s ² 5p ⁶ 5d6f	5s5p ⁶ 4f7p	5s5p ⁶ 8p	5s5p ⁵ 7p	5s5p ⁴ 7p
$5s^25p^64f^27g$	$5s^25p^65d7f$	5s5p ⁶ 4f8p	5s5p ⁶ 4f	5s5p ⁵ 8p	5s5p ⁴ 8p
$5s^25p^64f^28g$	5s ² 5p ⁶ 5d8f	5p ⁶ 4f ² 5d	5s5p ⁶ 5f	5s5p ⁵ 4f	5s5p ⁴ 4f
$5s^25p^54f^35d$	$5s^25p^54f^25d$		5s5p⁰6f	5s5p ⁵ 5f	5s5p ⁴ 5f
$5s^{2}5p^{3}4t^{3}6s$	5s ² 5r ⁵ 5 ⁴ 1 ² 6s		5.5-695	SSSP ⁹ 6f	5s5p*6f
SSSP [°] 4I [∗] 5°5 ^{°6} 4f ³ €∽	5s⁻5p°5d° 5s5p ⁶ 4f ³		383p°81 585p ⁵ 4£ ²	585p°/f 585p ⁵ 8f	585p ⁺ /f 585p ⁴ 8f
5s5p ⁶ 4f ³ 7p	$550p^{-41^{\circ}}$ $555n^{6}4f^{2}6n$		585p°41⁻ 585n ⁵ 4f6n	$585p^{2}01$ $585n^{4}4f^{2}$	585p ³ 4f ²
$5s5p^{6}4f^{3}8p$	$5s5p^{6}4f^{2}7n$		$5s5p^{-10p}$	$5s5p^{4}4f6n$	$5s5p^{3}4f6n$
P 0P	$5s5p^64f^28p$		5s5p ⁵ 4f8p	$5s5p^44f7p$	$5s5p^34f7p$
	1 - F		$5p^54f^25d$	5s5p ⁴ 4f8p	5s5p ³ 4f8p
			5p ⁶ 4f5d	5p ⁶ 5d	5p ⁵ 5d
				$5p^44f^25d$	5p ⁴ 4f5d
				5p°4f5d	

Table 3.14: Configurations included in HFR calculations for Pm V–X ions.

In Table 3.15, we give a summary concerning the number of levels and transitions for these ions by the HFR method. IPs, from NIST database (Kramida et al., 2024) are also mentioned as the levels calculated in HFR approach are below these IPs.

Table 3.15: Number of levels and transitions obtained in HFR calculations for Pm V–X. The ionization potentials are also given for each ion.

Ion	Number of levels ^a	Number of lines ^b	$IP (cm^{-1})^c$
Pm V	10 522	1 152 223	497 900
Pm VI	3 161	275 006	688 000
Pm VII	735	30 527	814 000
Pm VIII	3 447	619 269	939 000
Pm IX	7 826	1 130 215	1 116 000
Pm X	7 694	1 068 431	1 250 000

^t Total number of HFR levels selected below the IP considered in opacity calculations

^b Total number of transitions with HFR calculated $\log(gf)$ -values ≥ -5

^c Ionization potential taken from NIST (Kramida et al., 2024)

The MCDHF method was then applied to determine the radiative parameters for a sample of two representative Pm ions, namely Pm VI and Pm IX. The same methodology as the one developed in the previous sections was used. A set of configurations was used to gradually incorporate valence-valence (VV) and core-valence (CV) correlations for each of these ions. This strategy is shown in Table 3.16 where all allowed transitions were computed between the MR configurations, *i.e.* all considered as spectroscopic.

For Pm VI, the MR consisted of $5p^{6}4f^{2}$, $5p^{6}5d^{2}$ even- and $5p^{6}4f5d$, $5p^{5}5d^{3}$ odd-parity configurations. For this ion, orbitals 1s to 4f were optimized on the respective ground configurations (*i.e.* $5p^{6}4f^{2}$) while 5d orbital was optimized using the MR configurations, keeping all other orbitals fixed. Then, VV1 and VV2 models were built by adding SD excitations from 5s, 5p, 5d, 4f to 5s, 5p, 5d, 5f, 5g and to 6s, 6p, 6d, 6f, 5g active orbitals, respectively. From the latter, a CV model was then built by adding SD excitations from the 4d core orbital to the MR valence orbitals, namely 5s, 5p, 5d, and 4f. For Pm VI, it give rise to 142 859 and 842 073 CSFs, for the even- and odd-parities, respectively.

In the case of Pm IX, the MR was composed of the $5s^25p^34f^2$, $5s^25p^5$, $5s^25p^44f$ odd- and the $5s5p^6$, $5s5p^54f$, $5s^25p^45d$ even-parity configurations. The orbitals 1s to 4f were optimized on the $5s^25p^34f^2$ ground configuration while the 5d orbital was optimized using the MR configurations, keeping all other orbitals fixed. For this ion, a VV3 model in which the active set included 7s, 7p, 7d, 6f, and 5g orbitals was added to the VV1 and VV2 models detailed previously. From VV3, CV calculations were then carried out by allowing SD excitations from the 4d core orbital to 5s, 5p, 5d, 4f, 5f, and 5g, giving rise to 3 767 300 and 622 057 CSFs in the odd- and even-parities of Pm IX.

Calculation	Pm VI	Pm IX
MR	Even parity	Odd parity
	$5p^64f^2$	$5s^25p^34f^2$
	$5p^65d^2$	$5s^25p^5$
		$5s^25p^44f$
	Odd parity 5p ⁶ 4f5d 5p ⁵ 5d ³	Even parity $5s5p^6$ $5s5p^54f$ $5s^25p^45d$
VV1	$\{5s, 5p, 5d, 5f, 5g\}$	$\{5s, 5p, 5d, 5f, 5g\}$
VV2	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}
VV3	{7s,7p,7d,6f,5g}	{7s,7p,7d,6f,5g}
CV	{5s,5p,5d,4f}	{5s,5p,5d,5f,5g}
CSFs	984 932	4 389 357

Table 3.16: Computational strategies used in MCDHF calculations for Pm VI and Pm IX ions.

As mentioned in the beginning of this section, CI+MBPT method was not used for these ions since there are no experimental data available to guide the computation in the selection of the potential.

As for previous ions, we compared our HFR and MCDHF results. Such comparisons are illustrated in Figure 3.13 where the HFR oscillator strengths ($\log(gf)$ -values) are plotted as a function of results obtained using the MCDHF method for transitions involving the ground level from Pm VI and Pm IX ions. In that cases, we noted an overall good agreement, the average relative differences between HFR and MCDHF oscillator strengths being found to be within 25%.



Figure 3.13: Comparison between the oscillator strengths (log(gf)) computed in this work using HFR and MCDHF methods for lines involving the ground level in Pm VI and Pm IX ions.

3.1.6 Sm V–X ions

For Sm V–X ions, from an experimental point of view, there are no data available for these ions. It is therefore crucial to perform theoretical calculations to obtain radiative parameters for these ions. In order to compute the atomic structure and to determine spectroscopic parameters for Sm V-X ions, we used in a first step, the pseudo-relativistic Hartree-Fock (HFR) approach described by Cowan (1981). Regarding the previous described lanthanide ions, for every ion under consideration, configuration interactions were incorporated through multi-configurational expansions, considering the electronic correlation outside of a Pd-like ionic core, where 46 electrons occupied every subshell ranging from 1s to 4d. Outside this ionic core, the remaining k electrons (with k = 12, 11, 10, 9, 8, and 7 for Sm V, VI, VII, VIII, IX and X, respectively) were assumed to occupy mainly the 4f, 5s and 5p subshells while allowing some SD excitations towards more excited valence nl orbitals, with n < 8 and l < 4. No semi-empirical radial parameter adjustment was possible because there is no experimental data available for these ions. Nevertheless, as recommended by Cowan (1981), all Slater integrals (F^k , G^k , and R^k) were scaled down by a factor 0.90 to approximate the cumulative effect of the infinity of small perturbations caused by configurations not explicitly included in the HFR models. A summary of the list of configurations that were included in HFR calculations for Sm V-X ions is given in Table 3.17.

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$5s5n^64f^2$ $5n^54f^25d$ $5s5n^4Af6r$
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5s5p ⁴ 4f8r
5p ⁶ 5d
$5p^65d$ $5p^44f^25d$

Table 3.17: Configurations included in HFR calculations for Sm V–X ions.

In Table 3.18, we outlined the number of lines and levels below the IP taken from the NIST database (Kramida et al., 2024). It can be noted that a little more than 100 million radiative transitions were calculated when considering the six ions together.

Table 3.18: Number of lines, number of levels and ionization potentials used in opacity calculations of Sm V–X ions.

Ion	Number of levels ^a	Number of lines ^b	$IP (cm^{-1})^c$
Sm V	31 142	17 267 783	505400
Sm VI	13 006	5 426 148	700 000
Sm VII	14 495	10 245 968	830 000
Sm VIII	23 015	30 795 559	955 000
Sm IX	21 432	26 651 944	1 140 000
Sm X	18 852	12 813 888	1 276 000

^a Number of levels included in HFR calculations below IP

^b Number of lines with HFR calculated $\log(gf)$ -values \geq -5

^c IP taken from NIST database (Kramida et al., 2024)

To assess the precision of the HFR outcomes acquired in this study, we additionally conducted atomic structure computations employing the Multi-Configuration Dirac-Hartree-Fock (MCDHF) method (Grant, 2007). Two samarium ions were selected for this purpose, namely Sm VI and Sm VII. The MR was chosen in each of these ions to take into account the configurations from which the radiative transitions were calculated. Then, by adding SD excitations involving only valence electrons (*i.e.* outside the Pd-like $4d^{10}$ core) on the one hand, and between core and valence electrons on the other hand, valence-valence (VV) and core-valence (CV) correlations were taken into account.

Concerning Sm VI, the MR was composed of the $5s^25p^64f^3$, $5s^25p^64f5d^2$ odd- and $5s^25p^64f^25d$, $5s^25p^65d^3$ even-configurations. The orbitals from 1s to 4f were optimized on the ground configuration ($5s^25p^64f^3$) while 5d was optimized using all the MR configurations, keeping all other orbitals fixed. Two VV models were built by adding SD excitations from 5s, 5p, 5d, 4f to {5s, 5p, 5d, 5f, 5g} (VV1) and to {6s, 6p, 6d, 6f, 5g} (VV2) active sets. From the latter, a CV model was then built by adding SD excitations from the 4d core orbital to the MR valence orbitals, namely 5s, 5p, 5d and 4f. This gave rise to a total of 1 675 493 configuration state functions (CSFs) for both parities.

In the case of Sm VII, the $5s^25p^54f^3$, $5s^25p^64f^2$, $5s^25p^65d^2$ even- and the $5s^25p^64f5d$, $5s^25p^55d^3$ odd-configurations were included in the MR in which 1s to 4f and 5d orbitals were optimized on the ground configuration ($5s^25p^54f^3$) and on all MR configurations, respectively. In VV1 and VV2 models, SD excitations from MR orbitals to the {5s, 5p, 5d, 5f, 5g} and {6s, 6p, 6d, 6f, 5g} active sets were considered. A CV model was then built from VV2 by adding single excitations from 4d to 5s, 5p, 5d and 4f subshells (MR orbitals). This led to a calculation involving 1 581 536 CSFs for both parities together. Table 3.19 summarizes all the configurations and dimensions concerning these two Sm ions for MCDHF calculations.

Calculation	Sm VI	Sm VII
MR	Odd parity	Even parity
	$5s^25p^64f^3$	$5s^25p^54f^3$
	$5s^25p^64f5d^2$	$5s^25p^64f^2$
		$5s^25p^65d^2$
	Even parity	Odd parity
	$5s^25p^64f^25d$	$5s^25p^64f5d$
	$5s^25p^65d^3$	$5s^25p^55d^3$
VV1	{5s,5p,5d,5f,5g}	{5s,5p,5d,5f,5g}
VV2	{6s,6p,6d,6f,5g}	{6s,6p,6d,6f,5g}
CV	{5s,5p,5d,4f}	{5s,5p,5d,4f}
CSFs	1 675 493	1 581 536

Table 3.19: Computational strategies used in MCDHF calculations for Sm VI and Sm VII ions.

As mentioned in Table 3.18, Sm ions produce a very large number of spectral lines when including all the configurations listed in Table 3.17 in HFR method. Assessing the accuracy of the radiative parameters obtained for such a large number of transitions is undoubtedly illusory, but one can get a rough idea by contrasting our HFR data with those derived from the MCDHF calculations carried out in this work for these two specific ions, Sm VI and Sm VII. In order to do that, we perfomed a comparison for transitions involving the ground configurations $(5p^{6}4f^{3} \text{ for Sm VI and } 5p^{5}4f^{3} \text{ for Sm VII})$. We found a satisfactory overall agreement between the HFR gf-values and the MCDHF data obtained in the Babushkin gauge, the average ratios $gf_{\rm HFR}/gf_{\rm MCDHF}$ being equal to 0.88 and 0.99 for Sm VI and Sm VII, respectively, with a dispersion of the order of a factor of two in both cases. We also observed that, for the same transitions, the average differences between the MCDHF oscillator strengths calculated within the Coulomb and Babushkin gauges were approximately 30% (Sm VII) and 50% (Sm VI). Therefore, we will roughly assume that, for the most intense lines at least, the HFR oscillator strengths calculated in this work are accurate to within a factor of 2. For Sm VI and Sm VII, in this work, we only compared transitions involving the ground level because these configurations were used to optimize all orbitals, from 1s to 4f, in our MCDHF calculations. Additionally, it was really challenging to establish a clear relationship between the MCDHF and HFR results for other transitions.

An additional method of evaluating the reliability of our HFR gf-values is to take into account the cancellation factor (CF) (Cowan, 1981) associated to every computed transition. A very small value of this factor (usually less than 0.05) suggests that there may be more uncertainty affecting the corresponding oscillator strength. Our calculations confirmed that the CF was larger than 0.05 for the great majority of the strongest transitions (with $\log(gf) \ge -2$), which contributed the most to the opacity. Figure 3.14 provides an illustration of this, displaying the CF-values for each transition computed in Sm VI as a function of $\log(gf)$.



Figure 3.14: Cancellation factor (CF) for each Sm VI transition taken into consideration in the present work as a function of log(gf). The average CF as a function of oscillator strength is represented by the red curve, CF = 0.05 is represented by the green straight line, and the grey dots represent the CF-values obtained by HFR calculations for each of the transitions.

3.1.7 Eu V–VII to Lu V–VII

In this section, we provide atomic results for Eu V–VII to Lu V–VII. We do not talk about VIII to X charge state in this section since the atomic data with our computational methods were not been calculated. Indeed, for these latter ions, the extremely complex configurations (with open 5p and 4f subshells) lead, on the one hand, to very large Hamiltonian matrices which can be very challenging to diagonalize and, on the other hand, to a huge number of radiative transitions (up to several hundred millions) which are difficult to manipulate with the Cowan's code. This problem was overcome by the use of a statistical approach, described in the Chapter 5, making it possible to obtain the atomic data required to calculate the opacities.

For each ion considered in the present section, the configurations introduced in HFR computations are listed in Table 3.20. In the same table, we give the number of radiative transitions involving energy levels below the ionization potential and for which $\log(gf)$ -values ≥ -5 in our calculations. Using the ionization potentials from the NIST database (Kramida et al., 2024) it produced a total of approximately 800 million transitions for the entire set of ions that were taken into consideration in our work. The number of transitions for a single ion ranged from a few tens of thousands to a few tens of millions. As reminded in Section 2.1.6, the Slater integrals (F^k , G^k , and R^k) were scaled down by a factor of typically 0.90 in our HFR calculations in order to more accurately represent the experimental energy structure in the lanthanide ions taken into consideration.

For these ions, there is unfortunately no experimental data or theoretical data published yet, except for Yb V and Lu V, for which Meftah et al. (2013) (Yb V), Kaufman and Sugar (1978) (Lu V), and Ryabtsev et al. (2015) (Lu V) published experimental and theoretical levels and transitions. In this last section concerning atomic data, we propose a comparison between our theoretical (HFR and MCDHF) results for these two ions and also with the experimental data available in the literature.

Ion	Configurations	Number of lines
Eu V	5s ² 5p ⁶ 4f ⁵ , 5p ⁵ 4f ⁶ , 5p ⁶ 4f ³ 5d ² , 5p ⁶ 4f ³ 6s ² , 5p ⁶ 4f ⁴ nf $(n = 5 - 8)$, 5p ⁶ 4f ⁴ np $(n = 6 - 8)$, 5p ⁶ 4f ⁴ ns $(n = 6 - 8)$, 5p ⁶ 4f ⁴ nd $(n = 5 - 8)$, 5p ⁶ 4f ⁴ ng $(n = 5 - 8)$, 5p ⁵ 4f ⁵ 5d	39 109 459
Eu VI	5 $s^{2}5p^{6}4f^{4}$, $5s^{2}5p^{5}4f^{5}$, $5s^{2}5p^{6}4f^{2}5d^{2}$, $5s^{2}5p^{6}4f^{2}6s^{2}$, $5s^{2}5p^{6}4f^{2}5d6s$, $5s^{2}5p^{6}4f^{3}nf$ ($n = 5 - 8$), $5s^{2}5p^{6}4f^{3}np$ ($n = 6 - 8$), $5s^{5}5p^{6}4f^{4}nd$ ($n = 5 - 8$), $5s^{5}5p^{6}4f^{4}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}5d^{3}np$ ($n = 6 - 8$), $5s^{2}5p^{6}5d^{3}nd$ ($n = 5 - 8$), $5s^{2}5p^{6}5d^{3}nf$ ($n = 6 - 8$), $5s^{2}5p^{6}5d^{3}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{3}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{3}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{3}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{3}ng$ ($n = 5 - 8$), $5s^{2}5p^{6}4f^{3}ng$ ($n = 5 - 8$), $5s^{2}5p^{5}4f^{4}5d$, $5s^{2}5p^{5}4f^{4}ns$ ($n = 6 - 7$), $5s^{5}p^{6}4f^{4}np$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{2}5d6p$	37 939 936
Eu VII	5s ² 5p ⁶ 4f ³ , 5s ² 5p ⁶ 4f ² <i>n</i> f ($n = 5 - 8$)), 5s ² 5p ⁶ 4f ² <i>n</i> p ($n = 6 - 8$), 5s5 p ⁶ 4f ³ <i>n</i> d ($n = 6 - 8$), 5s5 p ⁶ 4f ³ <i>n</i> s ($n = 6 - 8$), 5s ² 5p ⁶ 5d ² <i>n</i> p ($n = 6 - 8$), 5s ² 5p ⁶ 5d ² <i>n</i> f ($n = 5 - 8$), 5s ² 5p ⁵ 4f ⁴ , 5s ² 5p ⁵ 4f ³ 6p , 5s ² 5p ⁶ 5d ³ , 5s ² 5p ⁵ 4f ³ 5d , 5s ² 5p ⁵ 4f ³ <i>n</i> s ($n = 6 - 8$), 5s ² 5p ⁶ 5d ² <i>n</i> d ($n = 6 - 8$), 5s ² 5p ⁶ 5d ² <i>n</i> s ($n = 6 - 8$), 5s ² 5p ⁶ 4f ² <i>n</i> d ($n = 5 - 8$), 5s ² 5p ⁶ 4f ² <i>n</i> s ($n = 6 - 8$), 5s ² 5p ⁶ 4f ² <i>n</i> g ($n = 5 - 8$), 5s5 p ⁶ 4f ⁴ <i>f</i> ⁴ , 5s5 p ⁶ 4f ³ <i>n</i> p ($n = 6 - 8$)	5 885 552
Gd V	$5s^{2}5p^{6}4f^{6}$, $5p^{5}4f^{7}$, $5p^{6}4f^{5}5f$, $5p^{6}4f^{5}6p$, $5p^{6}4f^{5}5g$, $5p^{6}4f^{5}5d$, $5p^{5}4f^{6}5d$	17 429 441
Gd VI	5 s^{2} 5 p^{6} 4 f^{5} , 5 p^{5} 4 f^{6} , 5 p^{6} 4 f^{3} 5 d^{2} ,5 p^{6} 4 f^{3} 6 s^{2} , 5 p^{6} 4 f^{4} <i>n</i> f (<i>n</i> = 5 - 8), 5 p^{6} 4 f^{4} <i>n</i> p (<i>n</i> = 6 - 8), 5 p^{6} 4 f^{4} <i>n</i> g (<i>n</i> = 5 - 8), 5 p^{6} 4 f^{4} <i>n</i> g (<i>n</i> = 5 - 8), 5 p^{5} 4 f^{5} 5 d	43 285 559
Gd VII	5s ² 5p ⁶ 4f ⁴ , 5s ² 5p ⁵ 4f ⁵ , 5p ⁵ 4f ⁴ 6p , 5s ² 5p ⁶ 4f ² 5d ² , 5s ² 5p ⁶ 4f ² 6p ² , 5s ² 5p ⁶ 4f ² 5d6 , 5s ² 5p ⁶ 4f ³ <i>n</i> f (<i>n</i> = 5 - 8), 5s ² 5p ⁶ 4f ³ <i>n</i> p (<i>n</i> = 6 - 8), 5s5p64f ⁴ <i>n</i> d (<i>n</i> = 5 - 8), 5s ⁵ 5p ⁶ 4f ⁴ <i>n</i> s (<i>n</i> = 6 - 8), 5s ² 5p ⁶ 5d ³ <i>n</i> p (<i>n</i> = 6 - 8), 5s ² 5p ⁶ 5d ³ <i>n</i> d (<i>n</i> = 5 - 8), 5s ² 5p ⁶ 5d ³ <i>n</i> f (<i>n</i> = 6 - 8), 5s ² 5p ⁶ 5d ³ <i>n</i> s (<i>n</i> = 6 - 8), 5s ² 5p ⁶ 4f ³ <i>n</i> g (<i>n</i> = 5 - 8), 5s ² 5p ⁶ 4f ⁴ 5d , 5s ² 5p ⁶ 4f ³ <i>n</i> g (<i>n</i> = 5 - 8), 5s ² 5p ⁵ 4f ⁴ 5d , 5s ² 5p ⁵ 4f ⁴ <i>n</i> s (<i>n</i> = 6 - 7), 5s5p ⁶ 4f ⁴ <i>n</i> p (<i>n</i> = 6 - 8), 5s ² 5p ⁶ 4f ² 5d 6 p	36 848 045
Tb V	$5s^25p^64f^7$, $5s^25p^54f^8$, $5s^25p^64f^65f$, $5s^25p^64f^66p$, $5s^25p^64f^65d$, $5s^25p^54f^75d$	19 732 305
Tb VI	$5s^25p^64f^6$, $5s^25p^54f^7$, $5s^25p^64f^55f$, $5s^25p^64f^56p$, $5s^25p^64f^55g$, $5s^25p^64f^55d$, $5s^25p^54f^65d$	22 760 992
Tb VII	5s ² 5p ⁶ 4f ⁵ , 5s ² 5p ⁵ 4 f ⁶ , 5s ² 5p ⁶ 4 f ³ 5d ² , 5s ² 5p ⁶ 4 f ³ 6s ² , 5s ² 5p ⁶ 4 f ⁴ <i>n</i> f ($n = 5 - 8$), 5s ² 5p ⁶ 4 f ⁴ <i>n</i> p ($n = 6 - 8$), 5s ² 5p ⁶ 4 f ⁴ <i>n</i> s ($n = 6 - 8$), 5s ² 5p ⁶ 4 f ⁴ <i>n</i> d ($n = 5 - 8$), 5s ² 5p ⁶ 4 f ⁴ <i>n</i> g ($n = 5 - 8$), 5s ² 5p ⁵ 4 f ⁵ 5d	44 951 913
Dy V	$5s^25p^64f^8$, $5s^25p^54f^9$, $5s^25p^64f^75f$, $5s^25p^64f^76p$, $5s^25s^25p^64f^75d$, $5p^54f^85d$	17 446 583
Dy VI	$5s^25p^64f^7$, $5s^25p^54f^8$, $5s^25p^64f^65f$, $5s^25p^64f^66p$, $5s^25p^64f^65d$, $5s^25p^54f^75d$	28 090 364
Dy VII	$5s^25p^54f^7$, $5s^25p^64f^6$, $5s^25p^64f^55f$, $5s^25p^64f^56p$, $5s^25p^64f^55g$, $5s^25p^64f^55d$, $5s^25p^54f^65d$	25 958 076
Ho V	$\begin{array}{llllllllllllllllllllllllllllllllllll$	25 784 469
Ho VI	$5s^25p^64f^8$, $5s^25p^54f^9$, $5s^25p^64f^75f$, $5s^25p^64f^76p$, $5s^25p^64f^75d$, $5s^25p^54f^85d$	25 463 893

Table 3.20: Configurations introduced in HFR for Eu V–VII to Lu V–VII.

Ion	Configurations	Number of lines
Ho VII	$5s^25p^64f^7$, $5s^25p^54f^8$, $5s^25p^64f^65f$, $5s^25p^64f^66p$, $5s^25p^64f^65d$, $5s^25p^54f^75d$	32 588 602
Er V	5 $5p^{6}4f^{10}$, $5s^{2}5p^{6}4f^{9}6p$, $5s^{2}5p^{6}4f^{9}7p$, $5s^{2}5p^{6}4f^{9}5f$, $5s^{2}5p^{6}4f^{9}6f$, $5s^{2}5p^{5}4f^{11}$, $5s^{2}5p^{5}4f^{10}5d$, $5s^{2}5p^{6}4f^{9}6s$, $5s^{2}5p^{6}4f^{9}7s$, $5s^{2}5p^{6}4f^{9}8s$, $5s^{2}5p^{6}4f^{9}5d$, $5s^{2}5p^{6}4f^{9}5d$, $5s^{2}5p^{6}4f^{9}5g$	22 183 496
Er VI	$ 5s^{2}5p^{6}4f^{9}, 5s^{2}5p^{6}4f^{8}6p, 5s^{2}5p^{6}4f^{8}7p, 5s^{2}5p^{6}4f^{8}5f, 5s^{2}5p^{6}4f^{8}6d, \\ 5s^{2}5p^{6}4f^{8}6s, 5s^{2}5p^{6}4f^{8}7s, 5s^{2}5p^{6}4f^{8}5d, 5s^{2}5p^{6}4f^{8}6d, \\ 5s^{2}5p^{5}4f^{9}5d $	27 351 536
Er VII	$5s^{2}5p^{6}4f^{8}$, $5s^{2}5p^{5}4f^{9}$, $5s^{2}5p^{6}4f^{7}5f$, $5s^{2}5p^{6}4f^{7}6p$, $5s^{2}5p^{6}4f^{7}5d$, $5s^{2}5p^{5}4f^{8}5d$	30 066 536
Tm V	5 $s^{2}5p^{6}4f^{11}$, 5 $s^{2}5p^{6}4f^{10}np$ ($n = 6 - 8$), 5 $s^{2}5p^{6}4f^{10}nf$ ($n = 5 - 8$), 5 $s^{2}5p^{5}4f^{12}$, 5 $s^{2}5p^{5}4f^{11}5f$, 5 $s^{2}5p^{5}4f^{11}6p$, 5 $s^{2}5p^{6}4f^{10}ns$ ($n = 6 - 8$), 5 $s^{2}5p^{6}4f^{10}nd$ ($n = 5 - 8$), 5 $s^{2}5p^{6}4f^{10}ng$ ($n = 5 - 8$), 5 $s^{2}5p^{5}4f^{11}nd$ ($n = 5 - 6$), 5 $s^{2}5p^{5}4f^{11}6s$	36 367 389
Tm VI	$5s^25p^64f^{10}$, $5s^25p^64f^96p$, $5s^25p^64f^97p$, $5s^25p^64f^95f$, $5s^25p^64f^96f$, $5s^25p^54f^{11}$, $5s^25p^54f^{10}5d$, $5s^25p^64f^96s$, $5s^25p^64f^97s$, $5s^25p^64f^98s$, $5s^25p^64f^95d$, $5s^25p^64f^96d$, $5s^25p^64f^97d$, $5s^25p^64f^95g$	23 160 749
Tm VII	5 $s^{2}5p^{6}4f^{9}$, 5 $s^{2}5p^{6}4f^{8}6p$, 5 $s^{2}5p^{6}4f^{8}7p$, 5 $s^{2}5p^{6}4f^{8}5f$, 5 $s^{2}5p^{6}4f^{10}$, 5 $s^{2}5p^{6}4f^{8}6s$, 5 $s^{2}5p^{6}4f^{8}7s$, 5 $s^{2}5p^{6}4f^{8}5d$, 5 $s^{2}5p^{6}4f^{8}6d$, 5 $s^{2}5p^{5}4f^{9}5d$	27 994 638
Yb V	$5s^{2}5p^{6}4f^{12}, 5s^{2}5p^{6}4f^{11}np (n = 6 - 8), 5s^{2}5p^{6}4f^{10}5d^{2}, \\5s^{2}5p^{6}4f^{10}6s^{2}, 5s^{2}5p^{6}4f^{10}5d6s, 5s^{2}5p^{6}4f^{11}nf (n = 5 - 8), \\5s^{2}5p^{5}4f^{13}, 5s^{2}5p^{5}4f^{12}5f, 5s^{2}5p^{5}4f^{12}np (n = 6 - 8), 5s^{2}5p^{6}4f^{11}ns \\ (n = 6 - 8), 5s^{2}5p^{6}4f^{11}nd (n = 5 - 8), 5s^{2}5p^{6}4f^{11}ng (n = 5 - 8), \\5s^{2}5p^{6}4f^{10}5d6p, 5s^{2}5p^{6}4f^{10}6s6p, 5s^{2}5p^{5}4f^{12}ns (n = 6 - 8), \\5s^{2}5p^{5}4f^{12}nd (n = 5 - 8), \\5s^{2}5p^{5}4f^{12}nd (n = $	26 053 560
Yb VI	$5s^{-}5p^{6}4f^{10}nd (n = 5 - 8)$ $5p^{6}4f^{11}, 5s^{2}5p^{6}4f^{10}np (n = 6 - 8), 5s^{2}5p^{6}4f^{10}nf (n = 5 - 8),$ $5s^{2}5p^{5}4f^{12}, 5s^{2}5p^{5}4f^{11}5f, 5p^{5}4f^{11}6p, 5s^{2}5p^{6}4f^{10}ns (n = 6 - 8),$ $5s^{2}5p^{6}4f^{10}nd (n = 5 - 8), 5s^{2}5p^{6}4f^{10}ng (n = 5 - 8), 5s^{2}5p^{5}4f^{11}nd$ $(n = 5 - 6), 5s^{2}5p^{5}4f^{11}6s$	37 034 149
Yb VII	5 s^{2} 5 p^{6} 4 f^{10} , 5 s^{2} 5 p^{6} 4 f^{9} 6 p , 5 s^{2} 5 p^{6} 4 f^{9} 7 p , 5 s^{2} 5 p^{6} 4 f^{9} 5 f , 5 s^{2} 5 p^{6} 4 f^{9} 6 f , 5 s^{2} 5 p^{5} 4 f^{11} , 5 s^{2} 5 p^{5} 4 f^{10} 5 d , 5 s^{2} 5 p^{6} 4 f^{9} 6 s , 5 s^{2} 5 p^{6} 4 f^{9} 7 s , 5 s^{2} 5 p^{6} 4 f^{9} 5 d , 5 $s^$	15 209 723
Lu V	5 $s^{2}5p^{6}4f^{13}$, $5s^{2}5p^{6}4f^{12}np$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{11}5d^{2}$, $5s^{2}5p^{6}4f^{11}6s^{2}$, $5s^{2}5p^{6}4f^{11}5d6s$, $5s^{2}5p^{6}4f^{12}nf$ ($n = 5 - 8$), $5s^{2}5p^{5}4f^{14}$, $5s^{2}5p^{5}4f^{13}5f$, $5s^{2}5p^{5}4f^{13}np$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{12}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{12}nd$ ($n = 5 - 8$), $5s^{2}5p^{6}4f^{12}ng$ ($n = 5 - 8$), $5s^{2}5p^{6}4f^{11}5d6p$, $5s^{2}5p^{6}4f^{11}6s6p$, $5s^{2}5p^{5}4f^{13}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{11}5d6p$, $5s^{2}5p^{6}4f^{11}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{11}5d6p$, $5s^{2}5p^{6}4f^{11}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{11}ns$	3 310 355
Lu VI	5 $5s^{2}5p^{6}4f^{12}$, $5s^{2}5p^{6}4f^{11}np$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{10}5d^{2}$, $5s^{2}5p^{6}4f^{10}6s^{2}$, $5p^{6}4f^{10}5d6s$, $5s^{2}5p^{6}4f^{11}nf$ ($n = 5 - 8$), $5s^{2}5p^{5}4f^{13}$, $5s^{2}5p^{5}4f^{12}5f$, $5s^{2}5p^{5}4f^{12}np$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{11}ns$ ($n = 6 - 8$), $5s^{2}5p^{6}4f^{11}nd$ ($n = 5 - 8$), $5s^{2}5p^{6}4f^{11}ng$ ($n = 5 - 8$), $5s^{2}5p^{6}4f^{10}5d6p$, $5s^{2}5p^{6}4f^{10}6s6p$, $5s^{2}5p^{5}4f^{12}ns$ ($n = 6 - 8$), $5s^{2}5p^{5}4f^{12}nd$ ($n = 5 - 8$)	30 620 917
Lu VII	5 $5p^{5}4f^{11}$, $5p^{6}4f^{10}np$ ($n = 6 - 8$), $5p^{6}4f^{10}nf$ ($n = 5 - 8$), $5p^{5}4f^{12}$, $5p^{5}4f^{11}5f$, $5p^{5}4f^{11}6p$, $5p^{6}4f^{10}ns$ ($n = 6 - 8$), $5p^{6}4f^{10}nd$ ($n = 5 - 8$), $5p^{6}4f^{10}ng$ ($n = 5 - 8$), $5p^{5}4f^{11}nd$ ($n = 5 - 8$), $5p^{5}4f^{11}ns$ ($n = 5 - 8$), $5p^{5}4f^{11}ns$	33 862 758

Table 3.20: Continued.

Concerning Yb V, Meftah et al. (2013) identified 1 080 lines using a sliding spark source, namely the 10 m high resolution vacuum ultraviolet normal-incidence spectrograph of the Meudon Observatory. The 13 energy levels concerning the ground configuration ($4f^{12}$) were determined by the spectrum analysis as well as the excited configurations ($4f^{11}$ 5d, $4f^{11}$ 6s and $4f^{11}$ 6p) which revealed 174, 12, and 43 levels, respectively.

We thus compared our HFR results with the Meftah et al. (2013) ones and found a very good agreement between their experimental wavelengths and our wavelengths determined by HFR calculations, *i.e.* the mean deviation $\Delta \lambda / \lambda_{exp}$ was found to be equal to 0.018 \pm 0.044.

In addition to the HFR calculations, we performed MCDHF calculations for Yb V. The MR set of configurations was chosen to include the $5p^{6}4f^{12}$, $5p^{6}4f^{11}6p$ even- and the $5p^{6}4f^{11}5d$, $5p^{6}4f^{11}6s$ odd-parity configurations. Orbitals from 1s to 4f were optimized on all the levels of the $5p^{6}4f^{12}$ ground configuration keeping all other orbitals fixed. A valence-valence (VV) model was then built by adding SD excitations from 6s, 6p, 5d, 4f to all orbitals up to 6s, 6p, 5d, 5f, 5g. For the correlation orbitals 5f and 5g, they were optimized on all the levels of the MR configurations. From the VV model, core-valence (CV) interactions were considered by adding SD excitations from the 4d core orbital to the MR valence orbitals, namely 6s, 6p, 5d, and 4f. This gave rise to a total of 1 924 269 configuration state functions when considering both parities together.

The energy level values obtained in this CV model revealed a good agreement with the experimental data reported by Meftah et al. (2013), the mean deviation $\Delta E/E_{exp}$ (with $\Delta E = E_{MCDHF} - E_{exp}$) being found to be equal to -0.002 ± 0.040 .

The strongest Yb V lines (those with observed intensities greater than $100 \times 10^6 \text{ s}^{-1}$) were taken from Meftah et al. (2013) and listed in Table E.1 in Appendix E. For those lines, we also reported the values inferred from the transition probabilities (gA) computed by Meftah et al. (2013) and the oscillator strengths (log gf) obtained in the present work using HFR and MCDHF methods. The mean deviation between the two calculations was found to be 24%. Based on comparisons between these log(gf)-values, which are displayed in Figures 3.15 and 3.16, we can conclude that our HFR results are in good agreement with those obtained with the MCDHF approach results.

The average discrepancy between the values derived from Meftah et al. (2013) and our HFR oscillator strengths is around 5%. It is important to note that these comparisons were made by excluding transitions affected by significant cancellation effects in HFR calculations, *i.e.* for which the CF < 0.05. In Table E.1 in Appendix E, the transitions concerned are those located at $\lambda = 543.205$ (first line), 564.458 (second line), 571.235, 583.541, 589.608, 594.713, 802.074 (second line) and 1 709.796 Å. The line at 1 577.883 Å was also excluded from the HFR/MCDHF comparison because a very large discrepancy (more than a factor of two) was found between the MCDHF *gf*-values obtained using the Babushkin and the Coulomb gauges.



Figure 3.15: Comparison between the oscillator strengths (log(gf)) obtained in the current work using HFR method and those deduced from the gA-values published by Meftah et al. (2013).



Figure 3.16: Comparison between the oscillator strengths (log(gf)) obtained in the current work using HFR and MCDHF methods for Yb V.

As far as Lu V is concerned, Kaufman and Sugar (1978) classified 419 lines as transitions among 136 energy levels belonging to the $4f^{13}$, $4f^{12}5d$, $4f^{12}6s$ and $4f^{12}6p$ configurations on the basis of observations made from a sliding spark discharge using a 10.7 m normal incidence

spectrograph in the range of $500 - 2\ 100$ Å. Additionally, the previous work reported, computed energy levels obtained with a limited configuration interaction model by applying Racah algebra techniques and semi-empirical adjustment of radial integrals (Racah, 1942). More recently, Ryabtsev et al. (2015) performed parametric calculations in Lu V using HFR method. Ryabtsev et al. (2015) identified 7 new levels using 20 experimental lines from 563 – 978 Å by comparing their calculated transition probabilities with the line intensities taken from an unpublished line list of wavelengths initially considered by Kaufman and Sugar (1978). Notably, these authors only published the computed transition probabilities for these twenty transitions; no radiative rate for the several hundred other lines that were experimentally measured in Lu V has been published up to this point.

As for Yb V, we compared our HFR energy levels found using configurations listed in Table 3.20 for Lu V with the Kaufman and Sugar (1978) experimental ones. We found a good agreement with an average relative deviation $\Delta E/E_{exp}$ equal to 0.004 \pm 0.006. We also described the atomic structure of Lu V using the MCDHF method with GRASP2018. The MR was defined from the experimentally known configurations, *i.e.* $4f^{13}$, $4f^{12}5d$, $4f^{12}6s$ and $4f^{12}6p$, where orbitals from 1s to 4f were optimized on the 4f¹³ ground configuration while 5d, 6s and 6p were optimized on the $4f^{12}$ 5d, $4f^{12}$ 6s and $4f^{12}$ 6p configurations and all the other orbitals being frozen. After the MR computation, different valence-valence (VV) models, in which SD excitations of valence electrons were considered in order to generate the CSF expansions. A first VV model (VV1) was built by adding to the MR configurations, SD excitations from 4f, 5d, 6s, 6p to the {6s, 6p, 5d, 5f, 5g} active set. Only the new orbitals were optimized, the other ones being kept to their values obtained before. The same strategy was used to build the more elaborate valence-valence models, namely VV2 and VV3 in which the {6s, 6p, 6d, 6f, 5g} and {7s, 7p, 7d, 6f, 5g} active sets were considered, respectively. These calculations gave rise to 415 613 (VV1), 1 327 923 (VV2) and 2 253 529 (VV3) CSFs when considering both parities together. Finally, from the VV3 model, a CV model was built by adding SD excitations from the 5s and 5p core orbitals to the unfilled subshells involved in the MR configurations, *i.e.*, 4f, 5d, 6s and 6p, allowing calculations including a total of 2 301 648 CSFs. The MCDHF energy level values found in our various models were confirmed to be in a good agreement with the available experimental data (Kaufman and Sugar, 1978; Ryabtsev et al., 2015). The mean relative deviations $\Delta E/E_{exp}$ (where $\Delta E = E_{MCDHF} - E_{exp}$) are found to be equal to 0.072 ± $0.017, 0.062 \pm 0.015, 0.031 \pm 0.014, 0.031 \pm 0.013$ and 0.011 ± 0.015 when moving from the simplest approximation (MR) to the most elaborate one (CV).

Table F.1 in Appendix F reports the oscillator strengths $(\log(gf))$ and transition probabilities (gA) calculated in this work with HFR and MCDHF methods for all the experimentally observed lines of Lu V that were taken from Ryabtsev et al. (2015) and Kaufman and Sugar (1978). Concerning HFR results listed in this Table, it was assessed that most of the HFR transition rates given in this Table were not affected by cancellation effects (transitions with a CF < 0.05 were indicated with * symbol in that Table). The results listed in Table F.1 for the MCDHF gA- and $\log(gf)$ -values were obtained with the CV model in the Babushkin gauge (which is equivalent to the length formalism in the non-relativistic limit). By comparing the data computed in the Coulomb gauge (velocity formalism) with the quantity dT defined by Ekman et al. (2014) as follows, one can assess the accuracy of these radiative rates:

$$dT = \frac{|A_B - A_C|}{\max(A_B, A_C)},$$
(3.1.2)

where A_B and A_C are transition probabilities in Babushkin and Coulomb gauges, given that for exact solutions of the Dirac equation, the electric dipole transition moment has the same value in both of these gauges (Grant, 1974). The transition moment varies for approximate solutions, and as a result, the dT parameter offers an indicator of the uncertainties surrounding the MCDHF transition probabilities and oscillator strengths. The average dT value for the transitions shown in Table F.1 was found to be 0.101 ± 0.111 , indicating that most of our MCDHF radiative rates are not more than 20% uncertain. The table indicates the few exceptions, or transitions for which the dT value is greater than 20% (annotated by # symbol in the Table). They only concern 38 lines among a total of 457.

The mean relative difference $\Delta A/\max(A_{\text{HFR}}, A_{\text{MCDHF}})$, where $\Delta A = A_{\text{HFR}} - A_{\text{MCDHF}}$, was found to be equal to -0.050 ± 0.498 , indicating a reasonable overall agreement between our HFR and MCDHF radiative rates for the entire set of transitions. Excluding the transitions for which CF < 0.05 and dT > 0.20 in HFR and MCDHF computations respectively, was found to improve the agreement between the two methods, as expected. The mean relative deviation was lowered to -0.012 ± 0.424 in this case. Figure 3.17 plots the HFR $\log(qf)$ -values as a function of the MCDHF ones to illustrate these comparisons. We point out that recent HFR and MCDHF calculations carried out in Lu IV showed a similar general agreement (Bokamba Motoumba et al., 2020). Larger differences could be expected for lower lutetium ionization stages given that it is more difficult to get a convergence of the results, especially when using the MCDHF method, for neutral and weakly-ionized atoms (II-IV). Finally, we found an average agreement of 31% and 56% for our HFR and MCDHF results, respectively, when comparing the data obtained in the present work with the qA-value calculated by Ryabtsev et al. (2015) for the 23 experimentally observed lines classified in their paper. Finally, it should be mentioned that the average agreement between HFR and MCDHF transition probabilities was found to be equal to 32%.



Figure 3.17: Comparison between the oscillator strengths (log(gf)) calculated in the present work using HFR and MCDHF methods for the experimentally identified spectral lines in Lu V. The top figure shows all the transitions and the bottom one includes only transitions for which CF > 0.05 and dT < 0.20 in HFR and MCDHF calculations, respectively. The dashed line represents the strict equality and the dotted lines correspond to an agreement of a factor two between both sets of results.

3.2 Ground states for La V–X to Sm V–X and Eu V–VII to Lu V–VII

From our HFR calculations described in the previous section, we have been able to deduce the ground state energy level for each ion of interest in this work which remains unclear in the literature. Some studies such as Kilbane and O'Sullivan (2010) and Banerjee et al. (2023) indicate ground configurations for moderately-ionized lanthanide atoms without mentioning the spectroscopic designation. Moreover, some ground configurations from those papers are not matching with the ones that we calculated with HFR. In the last section of this chapter, we propose a detailed comparison between the results coming from these studies and those from our work.

In Table 3.21, the ground state levels are listed for La V–X to Sm V–X ions. For lanthanum and cerium ions, the ground configurations calculated with HFR method agree with the ones listed in the NIST database and the ones from Kilbane and O'Sullivan (2010) as well as Banerjee et al. (2023) papers. It can be noticed, for Pm VII, Pm VIII, Sm VII and Sm VIII, ground configurations from the Kilbane and O'Sullivan (2010) paper are not in a good agreement with those listed in Banerjee et al. (2023) paper and ours. The former paper is based on HFR calculations. In this paper, in order to determine the ground level, they consider the lowest average energy of a configuration among all of the configurations introduced. Nevertheless, the ground state can have a lower energy than this average energy (*i.e.* the lowest average energy of a configuration among all of the ones introduced in the model) considered leading thus to an inadequate consideration of the ground configuration. Finally, although for Pr VII–X, Nd VI–X, Pm VI–X and Sm VII–X, the ground configurations found with the HFR method are not the same as the ones found in the NIST database, we confirm the recent results from the Banerjee et al. (2023) paper for most ions, the only exception occurring for Pm VII.

The difficulty of determining the ground configuration of such ions, namely Pr V–X, Nd V–X, Pm V–X and Sm V–X is related to the collapse of the 4f orbital. Indeed, for some lanthanide ions, configurations of the type $5s^25p^k$, $5s^25p^{k-1}4f$, $5s^25p^{k-2}4f^2$, $5s^25p^{k-3}4f^3$ are often strongly mixed and cross each other in the energy spectrum, leading even to modifications of the ground configurations along isoelectronic sequences. This is illustrated in Figure 3.18 where the HFR average energies are shown for Cs-like, Xe-like, I-like and Te-like ions.

Ζ	Ion	Ground configuration			Ground level	
		$NIST^a$	Kilbane ^b	Banerjee ^c	This work	This work
57	La V	5p ⁵	5p ⁵	5p ⁵	5p ⁵	${}^{2}P_{3/2}$
	La VI	$5p^4$	$5p^4$	$5\mathbf{p}^4$	$5\overline{p}^4$	${}^{3}P_{2}$
	La VII	$5p^3$	$5p^3$	$5\overline{p}^3$	$5p^3$	${}^{4}S_{3/2}$
	La VIII	$5p^2$	$5p^2$	$5p^2$	$5p^2$	${}^{3}P_{0}$
	La IX	5p	5p	5р	5p	${}^{2}\mathbf{P}_{1/2}$
	La X	$5s^2$	$5s^2$	$5s^2$	$5s^2$	${}^{1}S_{0}$
58	Ce V	$5p^6$	$5p^6$	$5p^6$	5p ⁶	${}^{1}S_{0}$
	Ce VI	$5p^5$	$5p^5$	$5p^5$	$5p^5$	${}^{2}\mathbf{P}_{3/2}$
	Ce VII	$5p^4$	$5p^4$	$5p^4$	$5p^4$	${}^{3}P_{2}$
	Ce VIII	$5p^3$	$5p^3$	$5p^3$	5p ³	${}^{4}S_{3/2}$
	Ce IX	$5p^2$	$5p^2$	$5p^2$	$5p^2$	$^{3}P_{0}$
	Ce X	5p	5p	5p	5p	${}^{2}\mathbf{P}_{1/2}$
59	Pr V	5p ⁶ 4f	5p ⁶ 4f	5p ⁶ 4f	5p ⁶ 4f	${}^{2}F_{5/2}$
	Pr VI	$5p^6$	$5p^6$	$5p^6$	$5p^6$	${}^{1}S_{0}$
	Pr VII	$5p^44f$	$5p^5$	$5p^5$	$5p^5$	${}^{2}\mathbf{P}_{3/2}$
	Pr VIII	5p ³ 4f	$5p^4$	$5p^4$	$5p^4$	${}^{3}P_{2}$
	Pr IX	$5p^24f$	$5p^3$	$5p^3$	$5p^3$	${}^{4}S_{3/2}$
	Pr X	$4f^2$	$5p^2$	$5p^2$	$5p^2$	${}^{3}P_{0}$
60	Nd V	$5p^64f^2$	$5p^64f^2$	$5p^64f^2$	$5p^64f^2$	${}^{3}\mathrm{H}_{4}$
	Nd VI	$5p^54f^2$	5p ⁶ 4f	$5p^64f$	$5p^64f$	${}^{2}F_{5/2}$
	Nd VII	$5p^44f^2$	$5p^6$	$5p^6$	$5p^6$	${}^{1}S_{0}$
	Nd VIII	$5p^34f^2$	$5p^5$	$5p^5$	$5p^5$	${}^{2}P_{3/2}$
	Nd IX	$5p^24f^2$	5p ³ 4f	$5p^3 4f$	$5p^34f$	${}^{5}F_{3}$
	Nd X	$5p4f^2$	$5p^24f$	$5p^24f$	$5p^24f$	${}^{4}G_{5/2}$
61	Pm V	$5p^64f^3$	$5p^64f^3$	$5p^64f^3$	$5p^64f^3$	${}^{4}I_{9/2}$
	Pm VI	$5p^54f^3$	$5p^64f^2$	$5p^64f^2$	$5p^64f^2$	${}^{3}\text{H}_{4}$
	Pm VII	$5p^44f^3$	$5p^64f$	$5p^54f^2$	$5p^{6}4f$	${}^{2}F_{5/2}$
	Pm VIII	$5p^34f^3$	5p ⁵ 4f	$5p^44f^2$	$5p^44f^2$	${}^{5}\mathrm{H}_{4}$
	Pm IX	$5p^24f^3$	$5p^34f^2$	$5p^34f^2$	$5p^34f^2$	${}^{6}H_{9/2}$
	Pm X	$5p4f^3$	$5p^24f^2$	$5p^24f^2$	$5p^24f^2$	${}^{5}I_{4}$
62	Sm V	$5p^{6}4f^{4}$	$5p^{6}4f^{4}$	$5p^{6}4f^{4}$	$5p^64f^4$	${}^{5}I_{4}$
	Sm VI	$5p^64f^3$	$5p^{6}4f^{3}$	$5p^{6}4f^{3}$	$5p^{6}4f^{3}$	${}^{4}I_{9/2}$
	Sm VII	$5p^44f^4$	$5p^{6}4f^{2}$	$5p^{5}4f^{3}$	$5p^{5}4f^{3}$	${}^{\mathrm{b}}\mathrm{H}_{3}$
	Sm VIII	$5p^{3}4f^{4}$	$5p^{5}4f^{2}$	$5p^44f^3$	$5p^44f^3$	${}^{\mathrm{o}}\mathrm{H}_{5/2}$
	Sm IX	$5p^24f^4$	$5p^34f^3$	$5p^34f^3$	5p ³ 4f ³	۲ <u>ا</u> 4
	Sm X	5p4f ⁴	$5p^24f^3$	$5p^24f^3$	$5p^24f^3$	^о К _{9/2}

Table 3.21: Ground configurations and ground levels of La V-X to Sm V-X ions.

^a Kramida et al. (2024)

^b Kilbane and O'Sullivan (2010)

^c Banerjee et al. (2023)



Figure 3.18: Calculated average energies for low-lying configurations in Cs-like, Xe-like, I-like and Te-like Pr, Nd, and Pm ions.

As for La V–X to Sm V–X, we also have been able to deduce the ground level for Eu V–VII to Lu V–VII ions. In Table 3.22, we compared the ground configurations obtained from our HFR models with those published previously by Kilbane and O'Sullivan (2010), Banerjee et al. (2023) and by the NIST database Kramida et al. (2024). For determining the ground states, they were systematically obtained with the whole set of configurations included in the physical models in HFR method, thus allowing all these configurations to influence the determination of the ground level. Banerjee et al. (2023) followed a different strategy using HULLAC code (Hebrew University Lawrence Livermore Atomic Code) developed by Bar-Shalom et al. (2001) to deduce the ground configurations in lanthanide ions. This study is based on the use of different ent central potentials in their HULLAC models calculated by changing the electron distribution in 4f and 5p orbitals and optimizing for energy levels belonging to different sets of configurations. It is worth mentioning that the 5s, 5p and 4f orbitals, which are very close to each other in the considered lanthanide ions, play a key role in determining the ground configuration. In our HFR calculations, these orbitals are different for each configuration. This gives confidence
in the designation of the ground state established on the basis of orbitals which are specific to the configuration to which they belongs. For most of the ions listed in this Table, we obtain the same results as the ones published by Banerjee et al. (2023). The only exception are for Pm VII (as mentioned earlier), Eu VII, Gd VII, Tb VII for which our calculations give ground configurations of the type $5p^{6}4f^{k}$, instead of $5p^{5}4f^{k+1}$ for Banerjee et al. (2023), with k = 1, 3, 4, 5, respectively. It is important to note that the ground configurations for two of these ions (Pm VII and Tb VII) that we calculated ($5p^{6}4f$ and $5p^{6}4f^{5}$) were not included in the theoretical models of Banerjee et al. (2023), whereas the ground configurations obtained by these authors were all included in the physical models that we took into consideration for all of the ions listed in Table 3.22. We also compared our results with the ones published by Kilbane and O'Sullivan (2010). Our results are in good agreement except for Dy VII.

We also compared our results with the ones available in the NIST database (Kramida et al., 2024) and noticed that the latter disagree with our results as well as with those of Kilbane and O'Sullivan (2010) and Banerjee et al. (2023) for many ions. This was to be expected given the relatively simple theoretical calculations (the majority of which date back to the 1970s), performed in various approximations (Carlson et al., 1970; Martin et al., 1978; Sugar and Kaufman, 1970; Rodrigues et al., 2004) and used to designate the ground levels for moderately- and highly-ionized lanthanides in the NIST compilation.

Ζ	Ion	Ground configuration			ı	Ground level
		$NIST^a$	Kilbane ^b	Banerjee ^c	This work	This work
63	Eu V	$5p^64f^5$	$5p^64f^5$	$5p^64f^5$	$5p^64f^5$	${}^{6}\text{H}_{5/2}$
	Eu VI	$5p^54f^5$	$5p^{6}4f^{4}$	$5p^64f^4$	$5p^64f^4$	${}^{5}I_{4}$
	Eu VII	$5p^44f^5$	$5p^64f^3$	$5p^54f^4$	$5p^64f^3$	${}^{4}I_{9/2}$
64	Gd V	$5p^64f^6$	$5p^{6}4f^{6}$	$5p^64f^6$	$5p^64f^6$	${}^{7}F_{0}$
	Gd VI	$5p^54f^6$	$5p^64f^5$	$5p^64f^5$	$5p^64f^5$	${}^{6}\mathrm{H}_{5/2}$
	Gd VII	$5p^44f^6$	$5p^{6}4f^{4}$	$5p^54f^5$	$5p^{6}4f^{4}$	${}^{5}\mathrm{I}_{4}$
65	Tb V	$5p^64f^7$	$5p^{6}4f^{7}$	$5p^64f^7$	$5p^{6}4f^{7}$	${}^{8}S_{7/2}$
	Tb VI	$5p^54f^7$	$5p^64f^6$	$5p^64f^6$	$5p^64f^6$	${}^{7}F_{0}$
	Tb VII	$5p^34f^8$	$5p^{6}4f^{5}$	$5p^54f^6$	$5p^{6}4f^{5}$	${}^{6}\mathrm{H}_{5/2}$
66	Dy V	$5p^64f^8$	$5p^64f^8$	$5p^64f^8$	$5p^64f^8$	${}^{7}F_{6}$
	Dy VI	$5p^54f^8$	$5p^{6}4f^{7}$	$5p^{6}4f^{7}$	$5p^{6}4f^{7}$	${}^{8}S_{7/2}$
	Dy VII	$5p^44f^8$	$5p^64f^6$	$5p^54f^7$	$5p^54f^7$	${}^{9}P_{5}$
67	Ho V	$5p^{6}4f^{9}$	$5p^{6}4f^{9}$	$5p^{6}4f^{9}$	$5p^{6}4f^{9}$	${}^{6}\mathrm{H}_{15/2}$
	Ho VI	$5p^54f^9$	$5p^64f^8$	$5p^64f^8$	$5p^64f^8$	$^{7}F_{6}$
	Ho VII	$5p^44f^9$	$5p^{6}4f^{7}$	$5p^{6}4f^{7}$	$5p^{6}4f^{7}$	${}^{8}S_{7/2}$
68	Er V	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	${}^{5}I_{8}$
	Er VI	$5p^{5}4f^{10}$	$5p^{6}4f^{9}$	$5p^64f^9$	$5p^64f^9$	${}^{6}\mathrm{H}_{15/2}$
	Er VII	$5p^44f^{10}$	$5p^{6}4f^{8}$	$5p^64f^8$	$5p^64f^8$	$^{7}F_{6}$
69	Tm V	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	${}^{4}I_{15/2}$
	Tm VI	$5p^{5}4f^{11}$	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	⁸ I ₈
	Tm VII	$5p^44f^{11}$	$5p^{6}4f^{9}$	$5p^64f^9$	$5p^64f^9$	${}^{6}\mathrm{H}_{15/2}$
70	Yb V	$5p^{6}4f^{12}$	$5p^{6}4f^{12}$	$5p^{6}4f^{12}$	$5p^{6}4f^{12}$	${}^{3}H_{6}$
	Yb VI	$5p^{5}4f^{12}$	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	${}^{4}I_{15/2}$
	Yb VII	$5p^44f^{12}$	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	$5p^{6}4f^{10}$	${}^{5}I_{8}$
71	Lu V	$5p^{6}4f^{13}$	$5p^{6}4f^{13}$	$5p^{6}4f^{13}$	$5p^{6}4f^{13}$	${}^{2}F_{7/2}$
	Lu VI	$5p^{6}4f^{12}$	$5p^{6}4f^{12}$	$5p^{6}4f^{12}$	$5p^{6}4f^{12}$	${}^{3}H_{6}$
	Lu VII	$5p^44f^{13}$	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	$5p^{6}4f^{11}$	${}^{4}I_{15/2}$

Table 3.22: Ground configurations and ground levels of Eu V–VII to Lu V–VII ions.

^a Kramida et al. (2024)

^b Kilbane and O'Sullivan (2010)

^c Banerjee et al. (2023)

Chapter 4

Astrophysical opacity calculations using pseudo- and fully-relativistic atomic data

In this chapter, we first explain the expansion formalism used to compute opacities. Then, astrophysical conditions necessary to compute opacities for lanthanide ions of interest in this work are detailed. After that, the influence of some important parameters such as cancellation factor (CF), scaling factor (SF), cut-off on oscillator strengths and the use of realistic partition functions instead of approximating the latter by only considering the statistical weight of the ground level on the computed opacity is also studied. Then, radiative parameters calculated and presented in Chapter 3 were used to compute opacities *via* the expansion formalism for all the lanthanide ions from the V to the VII charge state. The line-binned formalism is also explained and compared with the latter for a few ions of a specific lanthanide, namely Sm ions. Finally, Planck mean opacities are given for all the moderately-charged lanthanide ions, to find out the opacities of which elements are dominant depending on the temperature.

4.1 Expansion formalism

Kilonova light curves are highly dependent on the bound-bound opacity of the *r*-process element within the ejecta (Just et al., 2022). The matter is ejected at a high velocity and expands quickly in neutron star mergers. As a result, the photons gradually interact with spectral lines and undergo continuous redshift in a comoving frame. It is important to note that these lines are not exactly straight but rather widened by a number of processes, primarily thermal motion in the neutron star merger ejecta. The opacity is the average contribution from several lines within a particular wavelength range if the lines do not overlap, indicating that photons interacting with different lines are independent. Therefore, these bound-bound opacities can be evaluated using the expansion formalism (Karp et al., 1977; Eastman and Pinto, 1993; Kasen et al., 2006) according to which the contributions of a large number of lines to the monochromatic opacity are approximated by a discretization involving the summation of lines falling within a spectral width, while the radiative transfer is considered in the Sobolev (1960) approximation. More precisely, in this approach, the bound-bound opacity is calculated using the expression

$$\kappa^{bb}(\lambda) = \frac{1}{\rho ct} \sum_{l} \frac{\lambda_l}{\Delta \lambda} (1 - e^{-\tau_l}), \qquad (4.1.1)$$

where ρ (in g cm⁻³) is the density of the ejecta, c (in cm s⁻¹) is the speed of light, t (in s) is the elapsed time since ejection, λ (in Å) is the central wavelength within the region of width $\Delta\lambda$,

 λ_l are the wavelengths of the lines appearing in this range and τ_l are the corresponding optical depths. The latter are expressed using the following expression (Sobolev, 1960):

$$\tau_l = \frac{\pi e^2}{m_e c} f_l n_l t \lambda_l, \qquad (4.1.2)$$

where e (in C) is the elementary charge, m_e (in g) is the electron mass, f_l (dimensionless) is the oscillator strength, and n_l (in cm⁻³) is the density of the lower level of the transition. Since the local thermodynamic equilibrium (LTE) is assumed in this formalism (Pognan et al., 2022), n_l can be expressed using the Boltzmann distribution according to the statistical weight g_0 and the density n_0 of the ground state as

$$n_l = n_0 \frac{g_l}{g_0} e^{-E_l/k_B T}, (4.1.3)$$

where k_B is the Boltzmann constant (in cm⁻¹K⁻¹), T (in K) is the temperature and g_l and E_l (in cm⁻¹) are respectively the statistical weight (defined as $g_l = 2J_l + 1$, J_l being the total electronic angular momentum of the atom in the level l) and the energy (as measured with respect to the ground level) or the excitation potential of the lower level of the transition.

Summing Eq. (4.1.3) over all the levels of the considered ion, we obtain:

$$n = \sum_{l=0}^{\infty} n_l = \frac{n_0}{g_0} \sum_{l=0}^{\infty} g_l \ e^{-E_l/k_B T},$$
(4.1.4)

where n is the ion density, defined according to Banerjee et al. (2020) by the formula

$$n = \frac{\rho}{Am_p} X_j, \tag{4.1.5}$$

in which A is the mass number, m_p is the proton mass (in g) and X_j is the relative ionic fraction of the j^{th} ionization state. Introducing the partition function U(T) defined as

$$U(T) = \sum_{l=0}^{\infty} g_l \ e^{-E_l/k_B T},$$
(4.1.6)

Eq. (4.1.4) becomes

$$\frac{n_0}{g_0} = \frac{n}{U(T)}.$$
(4.1.7)

As a consequence, the Boltzmann distribution given by Eq. (4.1.3) can be written as

$$n_l = \frac{n}{U(T)} g_l \ e^{-E_l/k_B T},\tag{4.1.8}$$

and therefore Eq. (4.1.2) can read as:

$$\tau_l = \frac{\pi e^2}{m_e c} \frac{n\lambda_l t}{U(T)} g_l f_l e^{-E_l/k_B T}.$$
(4.1.9)

All the opacities presented in this work have been computed using a python code that we developed, enabling the consideration of the huge number of lines possible for each lanthanide ion.

4.2 Astrophysical conditions

In Eq. (4.1.1), some parameters are important to highlight, namely the density of the ejecta, ρ , the time post-merger, t, and the temperature, T, hidden in the Sobolev optical depth Eq. (4.1.2). Moderately-charged lanthanides (from V to X charge state) are expected to be present in early-phase kilonovae according to radiative transfer simulations (Banerjee et al., 2023). Typical early-phase kilonova ejecta conditions for t = 0.1 day post-merger are a density around $\rho = 10^{-10}$ g cm⁻³ and temperatures $T > 20\ 000$ K. Within the LTE assumption, the ionic fraction abundance for each species for a given temperature can be determined by using the Saha equation defined as:

$$\frac{n_j}{n_{j-1}} = \frac{U_j(T)U_e(T)}{U_{j-1}(T)n_e} e^{-\chi_{j-1}/k_B T},$$
(4.2.1)

where n_{j-1} is the density of the ion in the j-1 charge state, n_e is the electron density, χ_{j-1} is the ionization potential of the ion in the j-1 charge state, $U_j(T)$ and $U_{j-1}(T)$ are the partition functions of the ion in the j and j-1 charge states, respectively.

By executing a python code that we developed, we have been able to evaluate the partition functions corresponding to La V-X to Sm V-X by using our complete set of HFR levels in the Saha equation. These new partition functions, completed by those obtained for La I-IV to Sm I-IV by using the corresponding energy levels taken from the NIST database (Kramida et al., 2024) were incorporated into the Saha equation to determine the relative number of lanthanide atoms in different ionization stages, assuming a pure gas of the relevant lanthanide. In these calculations, we also included the relevant ionization potentials tabulated at NIST, mentioned in Table 3.2, 3.6, 3.9, 3.12, 3.15, 3.18, and electron densities estimated from the mass density of the kilonova ejecta, *i.e.* from $\rho = 10^{-13}$ g cm⁻³ to $\rho = 10^{-10}$ g cm⁻³ when going from the first ionization degrees (I-IV) to higher ones (V-X), as suggested by Gaigalas et al. (2019) and Banerjee et al. (2020), respectively. It allowed us to precisely know the temperatures corresponding to the maximum ionic abundance for each lanthanide considered in the present study. This is represented in Figures 4.1 to 4.6 showing the relative ionic fractions as a function of temperature. It can be seen from these Figures that the maximum abundance for a specific ionization degree are located around the same temperature regardless of the lanthanide considered, e.g. the maximum for the VII charge state is always around $T = 40\ 000$ K. In Table 4.1 all the temperatures for each maximum of abundances for moderately-charged lanthanide ions are given.



Figure 4.1: Relative ionic abundances for La I–X species as a function of temperature.



Figure 4.2: Relative ionic abundances for Ce I–X species as a function of temperature.



Figure 4.3: Relative ionic abundances for Pr I–X species as a function of temperature.



Figure 4.4: Relative ionic abundances for Nd I–X species as a function of temperature.



Figure 4.5: Relative ionic abundances for Pm I–X species as a function of temperature.



Figure 4.6: Relative ionic abundances for Sm I–X species as a function of temperature.

Spectra	La	Ce	Pr	Nd	Pm	Sm
V	25 000	24 600	25 000	24 000	24 000	24 700
VI	31 000	32 000	33 000	33 000	39 000	34 000
VII	38 000	39 000	40 000	40 000	42 000	42 000
VIII	45 000	45 000	45 000	47 000	49 000	49 000
IX	53 000	53 000	55 000	56 000	58 000	59 000
Х	62 000	66 000	68 000	65 000	67 000	68 000

Table 4.1: Temperatures (in K) corresponding to the maximum abundance for each of the moderately-charged lanthanide ions.

4.3 Impact of using realistic partition functions in Sobolev optical depth

In some papers from other groups (Gaigalas et al., 2019; Tanaka et al., 2020; Banerjee et al., 2020, 2022, 2023), the statistical weight of the ground level (q_0) is used instead of using the partition function in the evaluation of the Sobolev optical depths, namely in Eq. (4.1.9). That implies a major impact on the opacities as the partition function depends on the temperature while g_0 is independent from the latter. This can be illustrated in Figure 4.7 where the partition function U(T) is plotted as a function of the temperature T (K) for a typical lanthanide, namely Sm VII. For T larger than 20 000 K, *i.e.* typically conditions for early-phase kilonova ejecta where moderately-charged lanthanides are expected to be present, we can notice that there is almost two orders of magnitude of difference between g_0 and U(T). This largely impacts the opacity as it can be seen in Figure 4.8 where the blue curve corresponds to the opacity of Sm VII calculated by approximating the partition function U(T) by g_0 , and the green one represents the opacity of Sm VII obtained when using the partition function estimated taking all the energy levels deduced from our HFR calculations. The opacity obtained using $U(T) = g_0$ is overestimated, *i.e.* there is almost two orders of magnitude of difference. Consequently, using g_0 is inadequate for calculating opacities for these ions encountered in the ejecta of early-phase kilonovae.



Figure 4.7: Partition function U(T) of Sm VII as a function of the temperature using HFR data (orange) and the statistical weight of the ground state ($g_0 = 7$) of Sm VII (green)



Figure 4.8: Expansion opacities for Sm VII calculated with $\rho = 10^{-10}$ g cm⁻³, t = 0.1 d, T = 42~000 K using, respectively, the statistical weight of the ground state ($g_0 = 7$) (blue) and the partition function U(T) taking into account all the levels introduced in our HFR calculations (green).

4.4 Impact of atomic computations on the opacities

Before showing expansion opacities for moderately-charged (V–VII) lanthanides, it is important to show the influence of some parameters related to the atomic calculations on the opacities. In a first step, we studied the influence of oscillator strengths on opacities. Indeed, we show for a specific ion, Ce VI, the impact of taking transitions obtained with HFR method characterized by a $\log(gf) \ge -2$ (blue curve), $\log(gf) \ge -5$ (orange curve) and $\log(gf) \ge -6$ (green curve) in Figure 4.9. As it can be noticed from this Figure, the opacity reaches a convergence when all the transitions with $\log(gf) \ge -5$ are taken into account. There is, therefore, no need to calculate transitions with $\log(gf) \le -6$ (which increase the computational time as well as the memory size) since it induces marginal changes to the opacity. Because of this, all the transitions with $\log(gf) \ge -5$ involving energy levels below the ionization potentials. This convergence of expansion opacities is also highlighted in Fontes et al. (2020) who demonstrated in Figure 11 of their paper that, in the case of neutral neodymium, the opacities no longer varied when including transitions with $\log(gf) < -5$.



Figure 4.9: Expansion opacities of Ce VI for conditions such as $\rho = 10^{-10}$ g cm⁻³, t = 0.1 d and $T = 32\ 000$ K with transitions characterized by a $log(gf) \ge -2$ (blue), $log(gf) \ge -5$ (orange) and $log(gf) \ge -6$ (green).

We also studied the impact of the cancellation factor (CF) on opacities. Indeed, according to Cowan (1981), very small values of this factor (namely CF < 0.05) suggest that the corresponding transition rates should be taken with caution. Although these effects are limited to weak transitions (cf. Figure 3.14) we have examined their impact on the entire spectral range under consideration in this work. In order to do this, we compared in Figure 4.10 the opacities obtained using all the transitions (with $\log(gf) \ge -5$) calculated using HFR method with those deduced from transitions for which CF ≥ 0.05 . This Figure illustrates how the cancellation effects are spread fairly uniformly across the spectrum, suggesting that they are wavelength-independent. Consequently, the opacity calculations of the corresponding transitions does not significantly affect any particular spectral region, allowing the uncertainties on the computed atomic transition rates resulting from strong cancellation effects to be distributed uniformly across the opacities in the entire spectrum.



Figure 4.10: Expansion opacities of Nd IX for conditions such as $\rho = 10^{-10}$ g cm⁻³, t = 0.1 d and $T = 56\ 000$ K considering all the transitions (orange) and only transitions characterized by $CF \ge 0.05$ (blue).

The sensitivity of the opacities to the arbitrary scaling factor (SF) in HFR computations was also examined. In accordance with Cowan (1981)'s recommendation, which is discussed in Section 2.1.6, we multiplied all of the Slater electrostatic interaction integrals (F^k , G^k , and R^k) by a scaling factor of 0.90. We calculated the opacities with atomic data from HFR calculations, using scaling factors of 0.80, 0.85, and 0.95 to investigate the impact of this decision. We discovered that the choice of scaling factors (SF) in the atomic calculations did not significantly affect the overall properties of opacities, as shown in Figure 4.11, which compares the Nd IX opacities obtained using HFR atomic data with SF = 0.80, 0.85, 0.90, and 0.95.



Figure 4.11: Expansion opacities of Nd IX for conditions such as $\rho = 10^{-10}$ g cm⁻³, t = 0.1 d and $T = 56\ 000$ K using different scaling factors (0.80 in green, 0.85 in black, 0.90 in orange and 0.95 in blue).

Finally, since this work involved several MCDHF calculations for selected ions, namely La V, La VIII, La X, Ce V, Ce VIII, Ce X, Pr V, Pr X, Nd V, Nd VI, Pm VI, Pm IX, Sm VI, Sm VII, Yb V and Lu V, it was intriguing to look at the impact of the Babushkin (length) or Coulomb (velocity) gauges used in the oscillator strength calculations for a specific ion, namely Nd IX. The opacity of the latter obtained in both formalisms using the MCDHF radiative rates are compared in Figure 4.12. With the relative difference between the two calculations only exceeding a few percents in some specific cases corresponding to very low opacities at wavelengths larger than 7 000 Å, it is evident that the choice of gauge has no significant impact on the deduced opacities.



Figure 4.12: Expansion opacities of Nd IX for conditions such as $\rho = 10^{-10}$ g cm⁻³, t = 0.1 d and $T = 56\ 000$ K using MCDHF results (upper panel). Relative difference between both gauges (bottom panel).

4.5 Expansion opacities for La V–VII to Lu V–VII

After having discussed the influence of such parameters on the opacity, we calculated expansion opacities using HFR data for all lanthanides from V to VII charge states. We computed such opacities for different temperatures, namely T = 25000 K (Figure 4.13), 30000 K (Figure 4.14), 35000 K (Figure 4.15) and 40000 K (Figure 4.16) using a density of kilonova $\rho = 10^{-10}$ g cm⁻³ and a time post-merger t = 0.1 day. We chose these specific temperatures since the V spectrum of all lanthanide ions starts at T = 25000 K and the VII spectra ends around 40000 K (approximately as it is highlighted in Figures 4.1 to 4.6. The wavelength width $\Delta\lambda$ in Eq. (4.1.1) is chosen to be 1% of the wavelength at wavelengths greater than 1000 Å and $\Delta\lambda = 10$ Å for $\lambda < 1000$ Å.

In Figures 4.13 to 4.16, we can therefore see the opacity trend for each element depending on the temperature. At 25 000 K, Tb and Dy ions have the highest opacity at UV ranges reaching $10^2 \text{ cm}^2 \text{ g}^{-1}$ while Pr, Sm and Eu have the larger opacity in IR ranges reaching $10^{-2} \text{ cm}^2 \text{ g}^{-1}$. At 40 000 K, Tb and Dy are always predominant in UV ranges reaching an opacity of $10^3 \text{ cm}^2 \text{ g}^{-1}$ while their opacity decrease sharply in visible/IR to reach $10^{-4} \text{ cm}^2 \text{ g}^{-1}$. La and Ce ions have the highest opacity from visible to IR reaching $10^{-1} \text{ cm}^2 \text{ g}^{-1}$.



Figure 4.13: Expansion opacities for lanthanide elements at $T = 25\ 000\ \text{K}$ with $\rho = 10^{-10}\ \text{g cm}^{-3}$ and a time post-merger t = 0.1 day using $\Delta \lambda = 1\%$ of the wavelength at wavelengths greater than 1 000 Å and $\Delta \lambda = 10\ \text{Å}$ for $\lambda < 1000\ \text{Å}$.



Figure 4.14: Expansion opacities for lanthanide elements at $T = 30\ 000\ \text{K}$ with $\rho = 10^{-10}\ \text{g cm}^{-3}$ and a time post-merger t = 0.1 day using $\Delta \lambda = 1\%$ of the wavelength at wavelengths greater than 1 000 Å and $\Delta \lambda = 10\ \text{Å}$ for $\lambda < 1000\ \text{Å}$.



Figure 4.15: Expansion opacities of all lanthanides for $T = 35\ 000\ \text{K}$ with $\rho = 10^{-10}\ \text{g cm}^{-3}$ and a time post-merger t = 0.1 day using $\Delta \lambda = 1\%$ of the wavelength at wavelengths greater than 1 000 Å and $\Delta \lambda = 10\ \text{Å}$ for $\lambda < 1000\ \text{Å}$.



Figure 4.16: Expansion opacities for lanthanide elements at $T = 40\ 000\ \text{K}$ with $\rho = 10^{-10}\ \text{g cm}^{-3}$ and a time post-merger t = 0.1 day using $\Delta \lambda = 1\%$ of the wavelength at wavelengths greater than 1 000 Å and $\Delta \lambda = 10\ \text{Å}$ for $\lambda < 1000\ \text{Å}$.

4.6 Line-binned opacities

An alternative method for computing opacities is based on the line-binned formalism (Fontes et al., 2020). Within the latter, the opacity is calculated as:

$$\kappa_{bin}^{bb}(\nu) = \frac{\pi e^2}{\rho m_e c} \sum_{l} n_l f_l L_l(\nu),$$
(4.6.1)

where ν is the photon frequency, ρ is the mass density and $L_l(\nu)$ is the corresponding line profile function. From the continuous expression, a discrete formula of the opacity can be obtained by substituting $1/\Delta\nu$ for the line profile:

$$\kappa_{bin}^{bb}(\nu) = \frac{1}{\Delta\nu} \frac{\pi e^2}{\rho m_e c} \sum_{l \in \Delta\nu} n_l f_l, \qquad (4.6.2)$$

where $\Delta \nu$ represents the frequency width of a bin.

Eq. (4.6.2) is independent of the expansion time, which is an advantage over methods that assume a homologous flow, such as the expansion opacity approach. In conclusion, the two methods, namely the expansion opacity explained in Section 4.2 and the line-binned formalism provide the following relationship in terms of wavelength when the optical depth determined by Eq. (4.1.2) is taken into account:

$$\kappa^{bb} = \frac{1}{\Delta\lambda} \frac{1}{\rho ct} \sum_{l \in \Delta\lambda} \begin{cases} \lambda_l (1 - e^{-\tau_l}) & \text{for expansion opacity} \\ \lambda_l \tau_l & \text{for line-binned opacity.} \end{cases}$$
(4.6.3)

The expansion and line-binned opacities for Sm V–X ions were computed using the entire set of HFR atomic data obtained in this work in Section 3.1.6. In order to compare samarium expansion opacity with the one calculated at a temperature $T = 70\ 000$ K in Banerjee et al. (2022), it is important to consider Sm IX, such as Banerjee et al. (2022) did. Indeed, when looking at this

specific temperature ($T = 70\ 000\ \text{K}$) in Figure 4.17, Sm IX, Sm X and Sm XI has to be taken into account to compute opacities. The latter were thus calculated considering a density $\rho = 10^{-10}\ \text{g cm}^{-3}$ and a time after merger t = 0.1 day, as suggested by Banerjee et al. (2020) for the early phases of kilonovae in which Sm V–XI are expected to be present. The wavelength width appearing in Eq. (4.6.3) is chosen to be $\Delta\lambda = 10\ \text{Å}$. In Figure 4.18, we show the results obtained for four specific temperatures, namely $T = 25\ 000\ \text{K}$, 42 000 K, 50 000 K, and 70 000 K, the latter considered for comparison purposes with opacities published in Banerjee et al. (2022) at this specific temperature as mentioned before.

Over the whole wavelength range above 1 000 Å, there is good agreement between our expansion and line-binned opacities in all four cases. Below this threshold, the line-binned opacities are systematically higher by several orders of magnitude than the expansion opacities. At the lowest temperature considered ($T = 25\ 000\ K$), the differences are more noticeable than at the highest one ($T = 70\ 000\ K$). Fontes et al. (2020) and Banerjee et al. (2022) have already brought attention to these disparities. The latter work showed that, at far UV wavelengths, usually for $\lambda < 2\ 000\ Å$, the use of expansion opacities for lanthanides at 0.1 day post-merger should be considered cautiously. However, the same paper also stated that this limit was actually below the detection range of the existing UV instruments like Swift telescope (Roming et al., 2005).

We compared our opacity results with the ones published in the Banerjee et al. (2022) paper who performed expansion opacity calculations for three selected lanthanides, including samarium, up to the XI charge state, using new atomic data obtained from the HULLAC approach (Bar-Shalom et al., 2001). When comparing Banerjee et al. (2022) and our opacities, they show a maximum of $\kappa_{exp} \sim 3 \times 10^2$ cm² g⁻¹ and $\kappa_{exp} \sim 1.5 \times 10^2$ cm² g⁻¹ at $\lambda \sim 500$ Å respectively. A bump of the order of 10 cm² g⁻¹ and 2 cm² g⁻¹ at $\lambda \sim 1500$ Å is also observed for Banerjee et al. (2022) and our opacities, respectively. The opacity slowly decrease for longer wavelengths to reach, at $\lambda = 10000$ Å, values of about 10^{-3} and 10^{-2} cm² g⁻¹, in this work and in the Banerjee et al. (2022)'s paper, respectively. These differences are most likely explained by the fact that Banerjee et al. (2022) opacity computed with statistical weights of the ground levels, g_0 , are overestimated compared to ours which included more realistic partition functions (meaning our calculations are more accurate).

Lastly, estimating how sensitive the opacities found in this work are to the calculated radiative data is an interesting task. As mentioned in Section 3.1.6, we made the assumption that our HFR oscillator strengths were generally accurate to within a factor of two. It is clear from the Eq. (4.6.3) that this uncertainty has different effects on the expansion and line-binned opacities. In fact, an uncertainty of a factor 2 on the latter implies the same uncertainty on the opacity because the line-binned opacity is proportional to the sum of the oscillator strengths. Conversely, the uncertainty influencing the expansion opacity depends on the various f-values associated with the optical depth. More specifically, the uncertainty on the expansion opacity was estimated to vary between 35% (for gf = 1) and a factor of 2 (for $gf = 10^{-5}$) for an accuracy of a factor of 2 on the oscillator strengths.



Figure 4.17: Relative ionic abundances for Sm I–XI species as a function of temperature.



Figure 4.18: Expansion and line-binned opacities of Sm ions for $T = 25\,000, 42\,000, 50\,000$ and 70 000 K with a density $\rho = 10^{-10}$ g cm⁻³ and a time after merger t = 0.1 day and using $\Delta \lambda = 1\%$ of the wavelength at wavelengths greater than 1 000 Å and $\Delta \lambda = 10$ Å for $\lambda < 1\,000$ Å.

4.7 Planck mean opacities

As defined in Section 1.4, the Planck mean opacity is written as

$$\kappa^{\text{Planck}} = \frac{\int_0^\infty B(\lambda, T) \kappa_\lambda d\lambda}{\int_0^\infty B(\lambda, T) d\lambda},$$
(4.7.1)

where T is the temperature (K) and $B(\lambda, T)$ is the Planck (or black-body) function defined as

$$B_{\lambda,T} = \frac{2hc^2}{\lambda^5} \frac{1}{exp(\frac{hc}{\lambda kT}) - 1}.$$
(4.7.2)

When calculating the Planck mean opacities with the expansion opacities obtained in Section 4.5, we computed the relative contributions of the different lanthanide elements to the kilonova opacity between 25 000 and 40 000 K. This is reported in Figure 4.19 where the Planck mean opacity is plotted as a function of temperature for each of the lanthanides. In this Figure, we can notice that the opacity is dominated by Eu, Gd, Tb, Sm and Dy at 25 000 K while Tb, Dy, Gd, Ho and Eu are predominant at 40 000 K. On the other hand, the Planck mean opacity values for some lanthanide elements, like Ce, La, Pr, Lu, Pm, and Nd, are one order of magnitude (for $T = 40\ 000\ \text{K}$) to 2-3 orders of magnitude (for $T = 25\ 000\ \text{K}$) lower than those corresponding to the predominant elements mentioned above. These elements contribute very little to the mean opacity over the whole temperature range. The latter statement can be seen on Figure 4.20 where we computed the Planck mean opacity as a function of the atomic number Z for all lanthanides elements at $T = 25\ 000$ K and $T = 40\ 000$ K. We also compared our results with the ones presented by Banerjee et al. (2023). While the maximum value of the Planck mean opacity calculated in our work at 25 000 K agrees well with that inferred from Figure 5 of Banerjee et al. (2023), it is important to note that the maximum opacity obtained by these latter authors at 40 000 K is roughly three times greater than the result calculated in our work. Such a difference could be due to the differences in the physical models considered in the respective atomic calculations but also to the differences in the partition function calculations used for the estimation of expansion opacities as explained in Section 4.3.



Figure 4.19: Planck mean opacity for lanthanide elements between $T = 25\,000$ K and $T = 40\,000$ K.



Figure 4.20: Planck mean opacity for lanthanide elements between $T = 25\,000$ K and $T = 40\,000$ K as a function of Z.

Chapter 5

Atomic data and astrophysical opacities obtained from the Statistical Resolved Transition Array (RTA) method

This chapter introduces a statistical method originally developed by Bauche et al. (1991, 2015) to simulate atomic data for a given ion. This chapter is a crucial part of this work since the computational methods aforementioned show limitations for some specific lanthanide ions. To obtain atomic data computationally, it is necessary to solve the eigenvalue equation by diagonalizing the Hamiltonian matrix. However, for some lanthanides ions, namely for those whose degree of ionization is between the VIII-X, the matrix size exceeds the computational limits of our Cowan's code making the diagonalization impractical. It is thus extremely challenging to solve the eigenvalue equation. To overcome this issue, we investigated a statistical approach, the so-called Resolved Transition Arrays method (RTAs), which is based on a random-number method and uses the properties of the array to simulate the energies and intensities of the radiative lines in a realistic way. With this method, all the radial integrals appearing in compact formulae can be found by solving the atomic structure's radial parts, without the need of diagonalizing a big Hamiltonian matrix. The statistical approach can be used when the ion of interest is a chaotic system. Indeed, in such atoms composed by subshells within a huge number of electron with sufficient basis-state mixing, *i.e.* quantum-chaotic systems, the probability distribution of the line strength can be well approximated as uniform (Fujii and Berengut, 2020).

In the present chapter, we provide an extensive summary of the compact formulae (*ab initio* method) that are used to determine oscillator strengths, transition wavelengths, and energy levels required for the computation of expansion opacities. This method is applied to Sm VIII and Eu VI, two ions whose atomic data were already calculated with Cowan's code. The *ab initio* statistical RTA atomic parameters is validated through comparisons with HFR calculations and *a posteriori* statistical RTA calculations for such ions. Concerning the *a posteriori* approach, all parameters useful to simulate the energy levels, transition wavelengths and oscillator strengths are deduced from a full HFR calculation (*i.e.* the Hamiltonian is built and diagonalized). A comparison between the opacities obtained by the full HFR method and the RTA approach (*ab initio* and *a posteriori* methods) is also presented for the latter ions to finally apply the *ab initio* statistical method to Dy VIII, a complex ion challenging to treat with the Cowan's code.

5.1 Ab initio method

In order to calculate opacities using the expansion formalism explained in Section 4.1, we need to have access to energy levels, transitions wavelengths and oscillator strengths. These values can be drawn randomly in Gaussian distribution. Indeed, in Figure 5.1 (top panel) which is an example took from Bauche-Arnoult et al. (1985), all the lines from the spectra representing Kr^{9+} can be approximated by a Gaussian distribution. This array ($3d^84s - 3d^84p$) is called an Unresolved Transition Array (UTA). When highly-charged ions, such as Mo^{15+} or Pr^{32+} (middle and last panel) are considered, their lines can be represented by two different Gaussian distributions. The $3d^84s - 3d^84p$ array is then splitted into subarrays called Split-Orbit-Spin-Array (SOSA). Actually, this appears when the spin-orbit interaction becomes larger than Coulombian interactions, namely for moderately- or highly-charged ions. It is important to note that when the UTA is splitted into several peaks (SOSA), the same simulation has to be performed for each SOSA separately (Bauche et al., 2015) in order to determine the radiative parameters.



Figure 5.1: Samples of computed spectra in the $3d^84s$ - $3d^84p$ isoelectronic series (from Bauche-Arnoult et al. (1985)). With the exception of those whose strengths are less than 3% of the highest, all 401 lines are represented by heights that are proportionate to their strengths. These lines have all traditionally been increased to that 3% limit. The line spectra envelopes, for a given linewidth that is adequate for line coalescence, are represented by the dashed curves.

5.1.1 Energy levels

First, to compute energy levels, we need to calculate the total number of levels N_C of a configuration C. In order to do that, we have to compute the variance of the distribution of magnetic quantum number M of a configuration C. For an l^N configuration (Bauche et al., 2015):

$$v(l^{N}) = N \frac{4l - N + 2}{4l + 1} \frac{1}{12} (4l^{2} + 4l + 3),$$
(5.1.1)

where l is the azimuthal quantum number and N the number of electron for a given subshell. For more complex configurations, the general formula is:

$$v_M(C) = v(l^{N_1}l^{N_2}l^{N_3}) = v(l^{N_1}) + v(l^{N_2}) + v(l^{N_3}) + \dots$$
(5.1.2)

Once we have calculated the variance, the following compact formula Bauche et al. (2015) is used (using the approximation of a Gaussian distribution of magnetic quantum numbers M of a configuration C) depending on whether the configuration possesses an odd or an even number of electrons:

$$N_{C} = \frac{2g(C)}{\left[8\pi v_{M}(C)\right]^{1/2}} \begin{cases} \left[1 - \frac{1}{6v_{M}(C)} + \frac{\alpha_{4} - 3}{8}\right] & \text{odd} \\ \left[1 - \frac{1}{24v_{M}(C)} + \frac{\alpha_{4} - 3}{8}\right] & \text{even} \end{cases},$$
(5.1.3)

where α_4 is the kurtosis (flattening) coefficient (dimensionless) defined as μ_4^c/μ_2^c , the 4th centered moment over the 2nd centered moment, namely the variance. The α_4 is equal to 3 for Gaussian distributions, therefore, the last term in Eq. (5.1.3) vanishes. In Eq. (5.1.3), g(C) is the configuration degeneracy of C (Cowan, 1981) and is calculated as (Bauche et al., 2015):

$$g(C) = \prod_{i=1,n_C} \binom{4l_i + 2}{N_i},$$
(5.1.4)

where n_C is the total number of open subshells in C and N_i is the number of electrons in subshell *i*.

Using the corresponding statistical distribution (Gaussian distribution), N_C energy levels, E, are randomly selected for every electronic configuration C taken into consideration in our model. This Gaussian distribution *i.e.* for a configuration C can be written:

$$D_C(E) = \frac{N_C}{2\pi\sqrt{v_C}} \exp\left[-\frac{(E - E_{av})^2}{2v_C}\right],$$
(5.1.5)

where E_{av} is the average energy of the configuration C, a radial parameter (a linear combination of radial integrals) as defined in Eq. (8.9) in Cowan (1981), which can be determined by solving the set of radial wave equations for the electronic configuration C, here the pseudorelativistic Hartree–Fock equations (Cowan, 1981) and v_C is the variance of the distribution which is computed from compact formulae tabulated in Table (3.2) in Bauche et al. (2015). The latter depends upon products of Slater and spin-orbit radial integrals obtained with the same method as for the radial parameter E_{av} . The distribution of levels can also be calculated as a function of their total momentum quantum number J, $N_C(J)$. This is given by Bauche and Bauche-Arnoult (1987):

$$N_{C}(J) = \frac{g(C)}{v_{M}(C)(8\pi v_{M}(C))^{1/2}}(2J+1)\exp\left[-\frac{(2J+1)^{2}}{8v_{M}(C)} + \frac{\alpha_{4}-3}{24}\left(15(2J+1)-5\frac{(2J+1)^{3}}{2v}+\frac{(2J+1)^{5}}{16v^{2}}\right)\right],$$
(5.1.6)

where the term involving α_4 coefficient vanishes since $\alpha_4 = 3$ for Gaussian distributions. Since $N_C = \sum_J N_C(J)$, therefore, the random draw of $N_C(J)$ energy levels can be done using the distribution $D_C(E)$ presented in Eq. (5.1.5) for each value of J.

5.1.2 Transition wavelengths

Secondly, to compute the $L(C_u - C_l)$ transition wavelengths, λ_{lu} for each electric dipole (E1) line of a transition array $C_l - C_u$ between a lower configuration C_l and an upper configuration C_u of opposite parities, we use:

$$\lambda_{lu} = \frac{1}{\sigma_{lu}} = \frac{hc}{(E_u - E_l)},\tag{5.1.7}$$

where σ_{lu} is the wavenumber calculated with the difference between E_l and E_u which are respectively the level energy of the lower configuration C_l and the upper configuration C_u drawn randomly (as mentioned in Section 5.1.1) that obey to the E1 selection rules.

The total number of E1 lines of a $C_l - C_u$ array, $L(C_l - C_u)$, is calculated by (Bauche et al., 2015):

$$L(C_{l} - C_{u}) = \frac{3}{\sqrt{8\pi}} g(C_{l}) g(C_{u}) \left[v_{M}(C_{l}) + v_{M}(C_{u}) \right]^{-3/2} \times \left[1 - \frac{1}{v_{M}(C_{l}) + v_{M}(C_{u})} \right].$$
(5.1.8)

Eq. (5.1.3), Eq. (5.1.6) and Eq. (5.1.8) are an approximation explicitly written in Bauche et al. (2015) since there is no formulae existing for the total number of the levels of a configuration and for the total number of lines for a given E1 array, except in very simple cases such as the nl^2 configurations, where it is equal to (4l + 1), due to Pauli's principle (Bauche et al., 2015). These equations, written above, are therefore crucial to estimate both the number of levels and the number of lines when using the *ab initio* method.

5.1.3 Oscillator strengths

Finally, the weighted oscillator strength, $g_l f_{lu}$, of each E1 line belonging to a $C_l - C_u$ array are determined by Cowan (1981) such as:

$$g_l f_{lu} = (3.0376 \times 10^{-6}) \sigma_{lu} S_{lu}, \qquad (5.1.9)$$

where g_l is the statistical weight of the lowest level E_l of the transition, $\sigma_{lu} = E_u - E_l$ (in cm⁻¹) is obtained randomly following the procedure described in Section 5.1.1, and the line strength S_{lu} (in a.u.) is calculated by $S_{lu} = \eta (C_l - C_u) a_{lu}^2$ through a random value of the line amplitude

 a_{lu} Bauche et al. (1991) and a normalization factor $\eta(C_l - C_u) = S(C_l - C_u) / \sum_i a_{lu,i}^2$ where the total strength $S(C_l - C_u)$ of the $C_l - C_u$ array Bauche et al. (2015) is estimated as:

$$S(C_{l} - C_{u}) = S\left(n_{1}l_{1}^{N_{1}+1}n_{2}l_{2}^{N_{2}}n_{3}l_{3}^{N_{3}} - n_{1}l_{1}^{N_{1}}n_{2}l_{2}^{N_{2}+1}n_{3}l_{3}^{N_{3}}\right)$$

= $2l_{>}\binom{4l_{1}+1}{N_{1}}\binom{4l_{2}+1}{N_{2}}\binom{4l_{3}+2}{N_{3}}[P(n_{1}l_{1},n_{2}l_{2})]^{2},$ (5.1.10)

where $n_i l_i$ are open subshells, $l_>$ is the greater value between l_1 and l_2 and $P(n_1 l_1, n_2 l_2)$ is the E1 radial integral of r between the central-field monoelectronic radial function $R_{n_1 l_1}(r)/r$ and $R_{n_2 l_2}(r)/r$ as determined by solving the radial equation.

To simulate the transition amplitudes a_{lu} , they are drawn randomly in a Gaussian distribution centered at zero (in a.u) with a variance, v_a , correlated with the line wavenumber, σ_{lu} , from the following equation (Bauche et al., 1991):

$$\ln(v_a) = \alpha + \beta |\sigma - \sigma_{av}|, \qquad (5.1.11)$$

where σ is the average of the range boundaries $\sigma = (\sigma_1 + \sigma_2)/2$ where the values of σ_{lu} are distributed into consecutive ranges of equal widths in both sides of σ_{av} , the average wavenumber of the $C_l - C_u$ array.

The correlation parameters α and β appearing in Eq. (5.1.11) are determined using the following equations (Bauche et al., 1991). To calculate the value of β , one has to find the solution of the following implicit equation:

$$\left(X^2 + 1 - \frac{v_w}{v_{un}}\right) \exp\left(\frac{X^2}{2}\right) \operatorname{erfc}\left(\frac{X}{\sqrt{2}}\right) = X\sqrt{\frac{2}{\pi}},\tag{5.1.12}$$

where $X = -\beta \sqrt{v_{un}}$, while the value of α is deduced from X and from the average strength of the $C_l - C_u$ array, $S_{av}(C_l - C_u)$, as follows:

$$\alpha = \ln \left[S_{av}(C_l - C_u) \right] + \ln \left(X^2 + 1 - \frac{v_w}{v_{un}} \right) - \ln(X) + \frac{1}{2} \ln \left(\frac{\pi}{2} \right),$$
(5.1.13)

where $S_{av}(C_l - C_u) = S(C_l - C_u)/L(C_l - C_u)$, the former term of the fraction being expressed in Eq. (5.1.10) and the number of lines determined in Eq. (5.1.8).

In Eq. (5.1.12) and Eq. (5.1.13), v_{un} and v_w are respectively the unweighted and weighted variance of the line wavenumber σ_{lu} by the corresponding line strength S_{lu} . They can be evaluated by compact formulae for a $C_l - C_u$ UTA (Moszkowski, 1962; Bauche-Arnoult et al., 1979, 1982; Karazija and Rudzikaitė, 1988; Karazija, 1991).

5.2 A posteriori method

The *ab initio* statistical RTA atomic parameters and opacities were tested through comparisons with HFR calculations and *a posteriori* statistical RTA calculations. The latter method differs from the *ab initio* method in the sense that all parameters of the different distributions (energy levels and amplitudes) are directly determined from the atomic data obtained after diagonalization of the Hamiltonian matrix using the following formulae for the mean, Q_{av} , and the variance, v(Q), of a quantity Q obtained through diagonalization:

$$Q_{av} = \frac{\sum_{i} Q_i w_i}{\sum_{i} w_i},\tag{5.2.1}$$

$$v(Q) = \frac{\sum_{i} (Q_i - Q_{av})^2 w_i}{\sum_{i} w_i},$$
(5.2.2)

where Q_i can be the energy level E_i belonging to a configuration C or the wavenumber σ_{lu} of a transition belonging to a $C_l - C_u$ array and w_i is the weight that can be equal to 1 (unweighted moments) or equal to the corresponding level degeneracy g_i of a level E_i belonging to a configuration C or equal to the corresponding line strength S_{lu} of a transition belonging to a $C_l - C_u$ array (weighted moments). In this method, the correlation parameters α and β mentioned in the previous Eq. (5.1.11) are determined through a fitting procedure.

5.3 Sm VIII and Eu VI

For both lanthanide ions presented in this section, namely Sm VIII and Eu VI, opacities were computed using the expansion formalism as explained in Section 4.1.

Concerning Sm VIII, six configurations were included in our full HFR calculation: $5p^44f^3$, $5p^34f^36p$, $5p^54f^2$ for the odd- and $5p^34f^35d$, $5p^34f^36s$, $5p^34f^37s$ for the even-parity. There are six E1 transition arrays since the electric dipole transition operator is monoelectronic. The $5p^54f^2$ configuration was only included for configuration interaction (CI) purposes; it was not a part of any E1 transition array. Consequently, this configuration was not taken into account in our *a posteriori* and *ab initio* statistical RTA simulations.

For Eu VI, we have chosen to consider six configurations, namely $5p^64f^4$, $5p^54f^46p$, $5p^54f^5$ for the even- and $5p^54f^45d$, $5p^54f^46s$, $5p^54f^47s$ for the odd-parity, in our full HFR calculation, in our *a posteriori* and *ab initio* statistical RTA simulations. There are seven E1 transition arrays.

In the *a posteriori* statistical RTA simulations, we performed a statistical random draw considering both UTA and SOSA arrays since UTAs are splitted into SOSAs when the spin-orbit becomes larger. SOSAs can be seen as a model that provides a higher resolution of the atomic spectrum or a better wavelength distribution of the oscillator strengths. Consequently, we would expect that the opacity simulated by SOSAs would better reproduce the one obtained using HFR atomic radiative data. However, this is not always the case as it can be seen in Figure 5.2 where we compared opacity for a specific array in Sm VIII *i.e.* $5p^44f^3 - 5p^34f^35d$ using atomic data simulated using UTA and SOSA. It can be noticed that the UTA simulation matches better the HFR opacity than the one using SOSA arrays. A converse example is illustrated in Figure 5.3 where the SOSA simulation matches better the HFR opacity rather than considering UTA for the $5p^34f^36s - 5p^34f^36p$ array in Sm VIII. Because of this, we have decided to employ UTAs in all of our *ab initio* statistical RTA simulations since they require fewer statistical distributions (Bauche et al., 2015).



Figure 5.2: Expansion opacities computed in Sm VIII with $\rho = 10^{-10}$ g cm⁻³, t = 0.1 day and $T = 50\ 000$ K for the $5p^44f^3 - 5p^34f^35d$ array using the atomic data computed with the HFR method (blue curve), simulated with the a posteriori statistical RTA method considering SOSAs (orange curve) and considering a UTA (red curve).



Figure 5.3: Expansion opacities computed in Sm VIII with $\rho = 10^{-10}$ g cm⁻³, t = 0.1 day and $T = 50\ 000$ K for the $5p^34f^36s - 5p^34f^36p$ array using the atomic data computed with the HFR method (blue curve), simulated with the a posteriori statistical RTA method considering SOSAs (orange curve) and considering a UTA (red curve).

In Tables 5.1 and 5.2, we summarize for both ions, Sm VIII and Eu VI, the energy level distribution parameters, *i.e.* the average energy, E_{av} , the standard deviation, $\sqrt{v_C}$, and the number of levels, N_C , for each configuration in the *a posteriori* and in the *ab initio* RTA simulations. The latter have been obtained in collaboration with Dr. J-C. Pain.

Table 5.1: The average energy, E_{av} , standard deviation, $\sqrt{v_C}$ and total number of levels, N_C , are given for each configuration in Sm VIII as considered in the a posteriori and the ab initio statistical RTA calculations.

Configuration	$E_{av}^{a} ({ m cm}^{-1})$	$\sqrt{v_C} (\mathrm{cm}^{-1})$		N_C	
		A posteriori ^b	Ab initio ^{c}	A posteriori ^d	Ab initio ^e
$5p^44f^3$	78 888	38 958	40 705	589	620
$5p^34f^35d$	357 248	50 678	53 416	7 264	7 494
$5p^34f^36s$	484 513	42 286	44 007	1 549	1 603
$5p^34f^37s$	704 571	42 446	44 125	1 549	1 603
5p ³ 4f ³ 6p	556 742	43 581	45 289	4 547	4 711

^{*a*} HFR radial parameter (Section 5.1.1)

^b Calculated using Eq. (5.2.2).

^c Computed using HFR radial integrals and the compact formulae tabulated in Bauche et al. (2015) (5.1.1).

^{*d*} Determined by HFR calculations.

^e Computed using Eq. (5.1.3) in Section 5.1.1.

Table 5.2: Parameters of the statistical distribution of energy levels: the average energy, E_{av} , standard deviation, $\sqrt{v_C}$, and total number of levels, N_C , for each configuration in Eu VI as considered in both statistical RTA calculations, namely a posteriori and ab initio.

Configuration	$E_{av}^{a} ({\rm cm}^{-1})$	$\sqrt{v_C} \ (\mathrm{cm}^{-1})$		N_C	
		A posteriori ^b	Ab initio ^c	A posteriori ^d	Ab initio ^e
$5p^64f^4$	54 196	33 144	31 815	107	109
$5p^54f^45d$	311 979	43 820	45 703	5 756	5 930
$5p^54f^46s$	394 701	39 558	40 133	1 222	1 266
$5p^54f^47s$	559 456	39 664	40 214	1 222	1 266
$5p^54f^5$	148 108	40 991	42 095	1 168	1 199
$5p^54f^46p$	454 489	39 904	40 792	3 592	3 681
					-

^a HFR radial parameter (Section 5.1.1).

^b Calculated using Eq. (5.2.2).

^c Computed using HFR radial integrals and the compact formulae tabulated in Bauche et al. (2015) (Section 5.1.1).

^{*a*} Determined by HFR calculations

^e Computed using Eq. (5.1.3) (Section 5.1.1).

Regarding the standard deviation and the number of levels in both statistical methods, we noticed a very good agreement between them. The total number of levels for all the configurations considered in the E1 transition arrays for Sm VIII and Eu VI calculated *a posteriori* are respectively 15498 and 13065 whereas the *ab initio* values are 16031 and 13451. There is systematically more levels in the *ab initio* method than in *a posteriori* method since the latter is based on the HFR calculations in which only the levels below the ionization potential (IP) are considered while in the *ab initio* statistical RTA simulation all the levels from all the configurations considered are taken into account.

Moreover, for Sm VIII, when the $5p^54f^2$ configuration is considered in the full HFR calculation (with CI), the total number of levels is 15567. This configuration adds 69 levels contributing for

the configuration interaction (CI). Since this configuration was not considered in the E1 transition arrays in the *a posteriori* statistical RTA simulation, we therefore, did not include it in the Table 5.1.

Then, in Tables 5.3 and 5.4, a comparison between *a posteriori* and *ab initio* statistical RTA values is given for the number of lines, $L(C_l - C_u)$ and for the total strength, $S(C_l - C_u)$ for each $C_l - C_u$ array in Sm VIII and Eu VI, respectively. The *ab initio* values of the corresponding unweighted, $\sqrt{v_{un}}$, and weighted, $\sqrt{v_w}$, standard deviations of the wavenumber distribution, calculated by compact formulae, are also reported.

Table 5.3: Comparison between a posteriori and ab initio statistical RTA values for the number of lines, $L(C_l - C_u)$ and the total strength, $S(C_l - C_u)$, for each $C_l - C_u$ array in Sm VIII. The ab initio values of the corresponding unweighted, $\sqrt{v_{un}}$, and weighted, $\sqrt{v_w}$, standard deviations of the wavenumber distribution are also reported.

$C_l - C_u$ array	$L(C_l - C_u) \qquad \qquad S(C_l - C_u) \text{ (a.u)}$		_ι) (a.u.)	$\sqrt{v_{un}}^d$ (cm ⁻¹)	$\sqrt{v_w}^d$ (cm ⁻¹)	
	A posteriori ^a	Ab initio ^b	A posteriori ^a	Ab initio ^c		
$5p^44f^3 - 5p^34f^35d$	1 317 060	1 639 731	31 296	62 388	57 898	24 224
5p ⁴ 4f ³ – 5p ³ 4f ³ 6s	228 243	367 067	2 820	2 807	52 599	25 493
$5p^44f^3 - 5p^34f^37s$	253 897	367 067	333	332	52 723	26 714
$5p^34f^36p - 5p^34f^35d$	8 405 714	12 371 727	30 229	60 311	58 552	21 807
$5p^34f^36p - 5p^34f^36s$	1 656 733	2 757 175	92 920	92 679	32 533	9 054
$5p^34f^36p - 5p^34f^37s$	1 610 655	2 757 175	23 032	22 970	52 134	9 161

^a Determined after diagonalization of the Hamiltonian (HFR calculations).

^b Calculated using Eq. (5.1.8) (Section 5.1.2).

^{\circ} Calculated using Eq. (5.1.10) (Section 5.1.3).

^d Evaluated using the compact formulae of Bauche-Arnoult et al. (1979, 1982) (Section 5.1.3).

Table 5.4: Comparison between a posteriori and ab initio statistical RTA values for the number of lines, $L(C_l - C_u)$ and the total strength, $S(C_l - C_u)$, for each $C_l - C_u$ array in Eu VI. The ab initio values of the corresponding unweighted, $\sqrt{v_{un}}$, and weighted, $\sqrt{v_w}$, standard deviations of the wavenumber distribution are also reported.

$C_l - C_u$ array	$L(C_l -$	C_u)	$S(C_l - C_l)$	u) (a.u.)	$\sqrt{v_{un}}^d$ (cm ⁻¹)	$\sqrt{v_w}^d$ (cm ⁻¹)
	A posteriori ^a	Ab initio ^b	A posteriori ^a	Ab initio ^c		
$5p^{6}4f^{4} - 5p^{5}4f^{4}5d$	171 563	218 988	9 041	18 030	53 628	19 657
$5p^64f^4 - 5p^54f^46s$	38 098	48 569	851	849	51 726	23 181
$5p^{6}4f^{4} - 5p^{5}4f^{4}7s$	34 017	48 569	106	106	51 808	23 473
$5p^54f^5 - 5p^54f^45d$	1 640 627	2 324 253	7 783	23 291	51 714	18 690
$5p^54f^46p - 5p^54f^45d$	4735887	7 210 500	33 620	33 537	45 001	14 872
$5p^54f^46p - 5p^54f^46s$	900 390	1 589 407	91 797	91 553	31 610	6 248
$5p^54f^46p - 5p^54f^47s$	857 607	1 589 407	25 853	25 791	29 170	6 392

^a Determined after diagonalization of the Hamiltonian (HFR calculations).

^b Calculated using Eq. (5.1.8) (Section 5.1.2).

^c Calculated using Eq. (5.1.10) (Section 5.1.3).

^{*d*} Evaluated using the compact formulae of Bauche-Arnoult et al. (1979, 1982) (Section 5.1.3).

In the previous Tables, it is easy to notice that the number of lines calculated *ab initio* using Eq. (5.1.8) are systematically higher because there is no oscillator strength threshold, while in the *a posteriori* calculations based on the HFR atomic data calculations, we only considered transitions with a $\log(gf) \ge -5$. The total number of lines are respectively 13 536 304 for the

a posteriori statistical RTA simulation (without $5p^54f^2$), 14 287 901 for the full HFR calculation with CI (including $5p^54f^2$) and 20 259 942 for the *ab initio* statistical RTA simulation in Sm VIII. The number of lines for Eu VI are 8 378 185 (*a posteriori* simulation), 9 122 429 (HFR) and 13 029 693 (*ab initio* simulation). Regarding the total line strengths, results are in a good agreement except for the first ($5p^44f^3 - 5p^34f^35d$) and the fourth ($5p^34f^36p - 5p^34f^35d$) array in Sm VIII and for the first array ($5p^64f^4 - 5p^54f^45d$) and the fifth one ($5p^54f^46p - 5p^54f^45d$) in the case of Eu VI, where they differ by a factor two. These differences result from the weak lines that are missing from our *a posteriori* RTA simulations because of the threshold that was applied to the oscillator strengths.

Finally, the correlation parameters α and β and the average wavenumber σ_{av} values have to be calculated to randomly draw the amplitudes as described in Section 5.1.3. In Tables 5.5 and 5.6, we present a comparison between our *a posteriori* and *ab initio* statistical RTA values. Concerning the *a posteriori* RTA simulations, as we used SOSAs, except for the first array of Sm VIII and the fourth one of Eu VI, where UTAs were used instead, there are two or three α and β values per E1 transition array considered, depending if there are two or three SOSA peaks, while for the *ab initio* method, these parameters are calculated using UTAs (*i.e.* with a single value per E1 array). There are some differences in the α and β parameter values, but they are still in same order of magnitude. These are due to the fact that these parameters are least-square fitted in the *a posteriori* simulations while they are calculated exactly by Eq. (5.1.12) and Eq. (5.1.13) in the *ab initio* simulations.

$C_l - C_u$ array	σ_{av} (cn	n^{-1})	α		β (cı	β (cm)	
	A posteriori ^a	Ab initio ^b	A posteriori ^c	Ab initio ^d	A posteriori ^c	Ab initio ^e	
$5p^44f^3 - 5p^34f^35d$	324 611	329 727	-4.60	-1.94	-8.00E-5	-4.65E-5	
$5p^44f^3 - 5p^34f^36s$	390 379	410 223	-1.92	-3.73	-5.00E-5	-4.06E-5	
	437 841		-2.37		-4.00E-5		
$5p^44f^3 - 5p^34f^37s$	608 898	628 642	-5.85	-5.92	-8.00E-5	-3.75E-5	
	658 567		-5.95		-1.00E-4		
$5p^34f^36p - 5p^34f^35d$	162 556	205 030	-7.10	-3.86	-8.80E-5	-5.41E-5	
	209 851		-5.80		-1.00E-4		
$5p^34f^36p - 5p^34f^36s$	62 513	70 252	-2.10	-1.60	-1.50E-4	-1.41E-4	
	77 209		-1.70		-1.80E-4		
5p ³ 4f ³ 6p - 5p ³ 4f ³ 7s	142 597	149 861	-1.89	-2.49	-3.00E-4	-1.48E-4	
	157 545		-3.00		-2.50E-4		

Table 5.5: Comparison between a posteriori and ab initio statistical RTA values of the average wavenumber, σ_{av} , and the correlation parameters α and β for each $C_l - C_u$ array in Sm VIII.

^a Determined for UTA or each SOSA through diagonalization of the Hamiltonian (Section 5.2).

^b Determined for each UTA through compact formulae of Bauche et al. (2015) (Section 5.1.3).

^c Evaluated through a least-square fit procedure for each SOSA or UTA (Section 5.2).

^d Evaluated using Eq. (5.1.13) for each UTA (Section 5.1.3).

^e Evaluated using Eq. (5.1.12) for each UTA (Section 5.1.3).

$C_l - C_u$ array	σ_{av} (cm	n^{-1})	α	α		β (cm)	
	A posteriori ^a	Ab initio ^b	A posteriori ^c	Ab initio ^d	A posteriori ^c	Ab initio ^e	
$5p^{6}4f^{4} - 5p^{5}4f^{4}5d$	270 561	332 308	-6.10	-1.01	-3.50E-5	-6.21E-5	
	335 224		-3.45		-3.00E-4		
$5p^{6}4f^{4} - 5p^{5}4f^{4}6s$	327 444	344 245	-2.70	-2.81	-9.00E-5	-4.68E-5	
	371 089		-2.3		-1.14E-4		
$5p^{6}4f^{4} - 5p^{5}4f^{4}7s$	490 702	506 205	-4.15	-4.90	-1.10E-4	-4.60E-5	
	535 615		-4.20		-1.15E-4		
$5p^54f^5 - 5p^54f^45d$	168 695	173 574	-6.55	-3.09	-5.00E-5	-6.44E-5	
$5p^54f^46p - 5p^54f^45d$	59 261	144 941	-6.70	-3.76	-3.50E-5	-8.28E-5	
	99 735		-6.15		-1.30E-4		
	146 319		-5.00		-1.30E-4		
$5p^54f^46p - 5p^54f^46s$	52 553	59 041	-0.40	-0.69	-3.00E-4	-2.15E-4	
	63 230		-0.75		-1.99E-4		
$5p^54f^46p - 5p^54f^47s$	101 251	105 499	-0.90	-2.07	-2.70E-4	-2.08E-4	
	111 950		-4.20		-2.45E-4		

Table 5.6: Comparison between a posteriori and ab initio statistical RTA values of the average wavenumber, σ_{av} , and the correlation parameters α and β for each $C_l - C_u$ array in Eu VI.

^a Determined for UTA or each SOSA through diagonalization of the Hamiltonian (Section 5.2).

^b Determined for each UTA through compact formulae of Bauche et al. (2015) (Section 5.1.3).

^c Evaluated through a least-square fit procedure for each SOSA or UTA (Section 5.2).

^{*d*} Evaluated using Eq. (5.1.13) for each UTA (Section 5.1.3).

^e Evaluated using Eq. (5.1.12) for each UTA (Section 5.1.3).

After having calculated all these statistical parameters given in the previous Tables, we were able to simulate atomic data and use them to compute opacities for Sm VIII and Eu VI as shown in Figures 5.4 and 5.5. In these Figures, we compare the expansion opacities computed using the atomic data generated by the full HFR method (blue curve with CI and orange curve without CI) and by our a posteriori (red curve) and ab initio (green curve) RTA simulations for early-phase kilonova ejecta conditions 0.1 day after the merger, namely a density $\rho = 10^{-10}$ g cm^{-3} and a temperature $T = 50\ 000$ K and $T = 38\ 000$ K corresponding to the maximum ionic fraction of Sm VIII and Eu VI, respectively (as determined in Section 4.2). These conditions correspond to partition functions which were equal to 951 (a posteriori simulation), 1176 (ab initio simulation) and 1073 (HFR) in Sm VIII. Concerning Eu VI, the corresponding values were 307 (a posteriori simulation), 476 (ab initio simulation) and 316 (HFR). In addition to the opacity computations using HFR results with CI, we also computed opacities using atomic data generated by the full HFR method without CI (orange curve) in order to see the CI effect on our HFR opacities, which cannot be taken into account in the statistical RTA simulations. To do that, we intentionally set to zero all the Slater CI integrals R^k in Cowan's code in order to turn off the CI. As we can notice in these Figures, the orange curves (all $R^k = 0$), are in very good agreement with the ones obtained with the HFR atomic data including CI. Therefore, the latter, which are not taken into account in the statistical RTA simulations, can be neglected in the expansion opacity computations. Moreover, both statistical RTA simulations (a posteriori and *ab initio*) generate similar opacities as the ones computed with the HFR atomic data (with and without CI). Therefore, when standard computational atomic structure methods like HFR in Cowan's code are challenging to use, the *ab initio* statistical RTA method is an excellent way to calculate atomic data in order to compute expansion opacities for these complex ions in such conditions.



Figure 5.4: Expansion opacities in Sm VIII with $\rho = 10^{-10} \text{ g cm}^{-3}$, $t = 0.1 \text{ day and } T = 50\ 000 \text{ K}$ using the atomic data computed with the HFR method with configuration interaction (CI) (blue curve), without CI (orange curve), simulated with the a posteriori statistical RTA method (red curve) and with the ab initio statistical RTA method (green curve).



Figure 5.5: Expansion opacities in Eu VI with $\rho = 10^{-10}$ g cm⁻³, t = 0.1 day and $T = 38\,000$ K using the atomic data computed with the HFR method with configuration interaction (CI) (blue curve), without CI (orange curve), simulated with the a posteriori statistical RTA method (red curve) and with the ab initio statistical RTA method (green curve).

5.4 Dy VIII

Dy VIII is a highly complex lanthanide ion, characterized by a ground state $5p^44f^7$, with a half-filled 4f subshell. We chose to introduce six configurations in our model to represent the atomic structure of Dy VIII in our statistical RTA simulation, namely $5p^44f^7$, $5p^34f^8$ and $5p^34f^76p$ in the odd- and $5p^34f^75d$, $5p^34f^76s$ and $5p^34f^77s$ in the even-parity. The matrix of the Hamiltonian, even limited to two configurations (including the ground state and an excited configuration *e.g.* $5p^34f^75d$) has an enormous size since the excited configuration has 60 840 levels. Consequently, using our Cowan's code makes the diagonalization of the Hamiltonian unfeasible. As we have shown in the previous section that (*ab initio*) statistical RTA simulations can well reproduced the expansion opacities using the atomic data from HFR calculations, we can, thus, use this statistical method for this complex ion with confidence.

Table 5.7 and Table 5.8 contain all of the statistical parameters for the configurations and for the E1 transition arrays, respectively, useful to simulate atomic data. Considering all the configurations listed, the total number of levels is equal to 135 135. The issue of matrix size can be easily understood while looking at the huge number of levels per configurations, *e.g.* about 60 840 levels for $5p^34f^75d$. The total number of lines generated in Dy VIII reached the enormous number of 1 222 362 566. The α and β correlation parameter values and the average wavenumbers are given in Table 5.9 for each E1 transition array.

Table 5.7: Parameters of the statistical distribution of energy levels, $D_C(E)$, i.e. average energy, E_{av} , standard deviation, $\sqrt{v_C}$, and total number of levels, N_C , for each configuration in Dy VIII as considered in our ab initio statistical RTA calculation.

Configuration	$E^a_{av} (\mathrm{cm}^{-1})$	$\sqrt{v_C}^b (\mathrm{cm}^{-1})$	N_C^c
$5p^44f^7$	177 349	60 217	4 900
$5p^34f^75d$	487 912	86 490	60 840
$5p^34f^76s$	615 653	75 932	12 817
$5p^34f^77s$	850 623	76 133	12 817
$5p^34f^8$	244 778	59 859	5 740
5p ³ 4f ⁷ 6p	695 474	77 097	38 021

^{*a*} HFR radial integral (Section 5.1.1).

^b Computed using HFR radial integrals and the compact formulae tabulated in Bauche et al. (2015) (see Section 2.1).

² Computed using Eq. (5.1.3) Section 5.1.1).

Table 5.8: Ab initio statistical RTA values for the number of lines, $L(C_l - C_u)$, the total strength, $S(C_l - C_u)$), and the unweighted, $\sqrt{v_{un}}$, and weighted, $\sqrt{v_w}$, standard deviations of the wavenumber distribution for each $C_l - C_u$ array in Dy VIII.

$C_l - C_u$ array	$L(C_l - C_u)^a$	$S(C_l - C_u)^b$ (a.u.)	$\sqrt{v_{un}}^c$ (cm ⁻¹)	$\sqrt{v_w}^c (\mathrm{cm}^{-1})$
$5p^44f^7 - 5p^34f^75d$	89 978 658	520 824	40 198	16 451
$5p^44f^7 - 5p^34f^76s$	19 512 763	24 136	33 265	16 841
$5p^44f^7 - 5p^34f^77s$	19 512 763	2 855	33 128	17 110
$5p^34f^8 - 5p^34f^75d$	105 556 407	140 225	49 213	16 549
$5p^34f^76p - 5p^34f^35d$	689 477 967	533 565	37 459	15 388
$5p^34f^76p - 5p^34f^36s$	149 162 004	783 839	44 470	9 977
$5p^34f^76p - 5p^34f^37s$	149 162 004	207 009	27 986	10 202

^a Calculated using Eq. (5.1.8) (Section 5.1.2).

^b Calculated using Eq. (5.1.10) (Section 5.1.3).

 $^{^{\}circ}$ Evaluated using the compact formulae of Bauche-Arnoult et al. (1979, 1982) (Section 5.1.3).

$C_l - C_u$ array	$\sigma^a_{av} (\mathrm{cm}^{-1})$	$lpha^b$	β^c (cm)
$5p^44f^7 - 5p^34f^75d$	364 652	-3.80	-6.93E-5
$5p^44f^7 - 5p^34f^76s$	436 759	-5.96	-5.96E-5
$5p^44f^7 - 5p^34f^77s$	660 745	-7.77	-5.76E-5
$5p^34f^8 - 5p^34f^75d$	272 138	-5.04	-7.39E-5
$5p^34f^76p - 5p^34f^75d$	201 321	-5.81	-7.39E-5
$5p^34f^76p - 5p^34f^76s$	78 480	-3.20	-1.33E-4
$5p^34f^76p - 5p^34f^77s$	144 861	-5.09	-1.16E-4

Table 5.9: Ab initio statistical RTA values of the average wavenumber, σ_{av} , and the correlation parameters α and β for each $C_l - C_u$ array in Dy VIII.

^a Determined for each UTA through compact formulae of Bauche et al. (2015) (Section 5.1.3).

Evaluated using Eq. (5.1.13) for each UTA (Section 5.1.3).

^c Evaluated using Eq. (5.1.12) for each UTA (Section 5.1.3).

In Figure 5.6, the simulated expansion opacity of Dy VIII is illustrated using the same conditions than for Sm VIII, namely $T = 50\ 000$ K, $\rho = 10^{-10}$ g cm⁻³, t = 0.1 day. We can notice that the general trend is very similar to the one we observed in Figure 5.4 and Figure 5.5 for Sm VIII and Eu VI, respectively, with an opacity for the Dy VIII reaching a maximum of 4.85×10^3 cm² g⁻¹ around 285 Å.



Figure 5.6: Expansion opacities in Dy VIII with $\rho = 10^{-10}$ g cm⁻³, t = 0.1 day and $T = 50\ 000$ K using the atomic data simulated with the ab initio statistical RTA method.

The *ab initio* method, based on the RTA statistical approach, is thus an excellent method to simulate atomic data in order to compute expansion opacities for ions difficult to treat with traditional computational methods.

Conclusions and prospects

In this thesis, we have presented a new study of the atomic properties characterizing moderately-charged lanthanide ions, from 4+ to 9+ ionization degrees, in order to determine the opacities affecting the spectra emitted by early-phase kilonovae following neutron star mergers, *i.e.* for typical conditions 0.1 day after the merger, a density $\rho = 10^{-10}$ g cm⁻³ and a temperature $T > 20\ 000$ K.

To do this, the atomic structures and radiative data were obtained using large-scale calculations based on a multiplatform approach involving three different and independent theoretical methods, such as the pseudo-relativistic Hartree-Fock (HFR), the fully-relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) and the Configuration Interaction and Many-Body Perturbation Theory (CI+MBPT) methods. Such a multiplatform approach is the only way to estimate the precision of the results obtained through cross-comparisons between different computational procedures, especially when very little (if any) experimental data are available in the literature.

First of all, we calculated the atomic structures of La V–X to Sm V–X ions. For some of them, there are few experimental data available, namely for La V–X, Ce V–VIII, Ce X, Pr V, Pr X and Nd V. We computed atomic data for La V–X to Sm V–X by using the HFR method implemented in Cowan's code. In order to model the atomic structures, we explicitly introduced a large number of interacting configurations for each ion. When comparing the theoretical wavelengths with available experimental values, an overall good agreement was found for all the ions considered (< 6% for La and Ce ions and < 1% for Pr and Nd ions). Moreover, we compared our radiative data, such as oscillator strengths and transition probabilities, with experimental and theoretical data previously published in the literature for La IX, La X, Ce V, Ce VI, Ce VII, Ce VIII, Ce X, Pr V and Nd V. We noted a fairly satisfactory agreement for La IX, La X, Ce V, Ce VI and Nd V, the few significant discrepancies being attributed to the limited number of interacting configurations introduced in previous investigations. For the remaining ions, we noticed a good overall agreement (< 25% for Ce VII, Ce VIII and Ce X and < 15% for Pr V) since the theoretical data, from which we compared our results, are coming from more comprehensive theoretical frameworks.

The HFR results freshly obtained in the present work were then benchmarked with other computational methods to assess their reliability. More precisely, we computed the atomic structures and radiative parameters using the MCDHF method implemented in the GRASP2018 code and the CI+MBPT approach implemented in the AMBiT program for a sample of ions. In particular, MCDHF calculations were performed for La V, La VIII, La X, Ce V, Ce VIII, Ce X, Pr V, Pr X, Nd V, Nd VI, Pm VI, Pm IX, Sm VI and Sm VII ions. For each of those ions, we started by choosing a set of multi-reference (MR) configurations and gradually incorporated valencevalence (VV) and core-valence (CV) correlations. In a first step, we analyzed theoretical energy levels with the available experimental data and could find an overall good agreement (< 2% for La ions, < 5% for Ce V, < 1% for Ce VIII and Ce X, < 1% for Pr V and Nd V and < 12% Pr X). As regards the CI+MBPT method, the calculations were performed for La V, La VIII, La X, Ce V, Ce VIII, Ce X, Pr V, Pr X and Nd V. Nevertheless, since the CI convergence was found to be very slow for those ions, which makes it difficult to obtain atomic data, we rather used emu CI approach (except for Pr X and Nd V where CI+MBPT was used), implemented in AM-BiT package in order to reduce the size of the matrices without losing accuracy by considering only a few of the lowest-lying energy levels. We also compared our theoretical energy levels with the available data in the literature and noticed a good overall agreement (< 1% for La ions and Pr X, < 7% for Nd V, < 2% for Ce V and Ce VIII, < 5% for Ce X and < 3% for Pr V).

For both methods, MCDHF and emu CI (as well as CI+MBPT), we also cross-checked the accuracy of the oscillator strengths with the HFR results. We found some discrepancies due to the cancellation effects affecting the line strength calculations in HFR method and sometimes due to large disagreements between the length (Babushkin) and velocity (Coulomb) gauges in the MCDHF computations. However, these deviations were not found to be numerous enough to affect the global accuracy of the atomic data. Concerning Pm V-X and Sm V-X, since there are no experimental data available, it was therefore not possible to make a comparison. Despite this, we calculated their atomic structures by using MCDHF method in order to verify the accuracy of HFR oscillator strengths for transitions involving the ground levels. While we found a good agreement for Pm ions, we noticed slightly larger discrepancies in the case of Sm VI and Sm VII ions. This is mainly due to the differences in the Coulomb and Babushkin gauges in MCDHF method, namely 30% (Sm VII) and 50% (Sm VI). Finally, large-scale HFR atomic structure calculations were carried out in Eu V-VII to Lu V-VII ions. In this sample of ions, experimental and theoretical levels and transition rates were only published for Yb V and Lu V. Concerning the latter, we found a very good agreement when comparing our calculated wavelengths with the experimental data (within < 1% on average). For Yb V, the HFR oscillator strengths were also compared with experimental ones, showing a deviation of 5% for the most intense lines. We also cross-checked our HFR and MCDHF results and found a mean deviation of 24%.

Among the numerous results obtained in our calculations, a first interesting piece of information was the establishment of the ground configurations and the ground levels corresponding to all the lanthanide ions considered. It is indeed important to remember that this information was far from being known with certainty until now, the various predictions published previously often being in disagreement with each other, since they are based on other methods, often based on fairly limited theoretical models.

Thanks to the very large number of new atomic data obtained by means of the HFR method, the reliability of which was validated by the numerous comparisons mentioned above, these data were used to determine the astrophysical opacities corresponding to moderately-charged lanthanide ions, namely La V–VII to Lu V–VII. These ionization stages correspond to early-phase kilonova ejecta conditions expected a few hours ($\simeq 0.1$ day) after a neutron star merger when the density and temperature of the ejected matter are typically $\rho \simeq 10^{-10}$ g cm⁻³ and $T > 20\ 000$ K, respectively. Thus, the expansion opacities and the Planck mean opacities were determined using several hundred million radiative transitions in all the lanthanide ions of interest.

During these calculations, we highlighted the importance of including realistic partition functions (*i.e.* based on the consideration of the largest possible number of energy levels) for reliable estimation of opacities, instead of simply using the statistical weight of the ground level, as it was done in several opacity calculations previously published in the literature. In addition, we noticed that the relative contributions of lanthanide ions are wavelength- and temperature dependent. For example, at $T = 40\ 000\ K$, Tb and Dy are predominant at UV ranges while they decrease sharply at larger wavelengths to let Ce and La predominate. We also computed Planck mean opacities as a function of the temperature and noticed that Eu and Gd dominate at 25 000 K while Tb and Dy are predominant at 40 000 K. In the specific case of Sm ions, we also compared the expansion opacities with the ones obtained from the so-called line-binned formalism, sometimes used by other authors. Such a comparison only showed some differences in the UV range (typically below 2000 Å) for each temperature considered but it is worth mentioning that this wavelength region is located below the detection range of the existing UV instruments like Swift.

For some atomic systems, major difficulties may arise in carrying out theoretical calculations. This was the case for Eu VIII-X to Lu VIII-X lanthanide ions. In fact, the latter are characterized by very complex configurations with unfilled 4f and 5p subshells, resulting to very large Hamiltonian matrices which are often extremely difficult to diagonalize. For such ions, we developed a computational strategy based on a statistical approach, that is the so-called Resolved Transition Array (RTA), making it possible to obtain the atomic data required to estimate the corresponding opacities. In order to do that, we chose to apply this statistical approach to Sm VIII and Eu VI, two ions for which we have already computed the opacities using the atomic data obtained using the full HFR method (*i.e.* with diagonalization of the Hamiltonian). In light of the good agreement between opacities calculated with HFR results (actual HFR atomic data) and the ones calculated with the simulated data (statistical a posteriori and ab initio approach), we decided to apply the RTA method to Dy VIII, a complex ion challenging to treat with the HFR computational procedure. By using compact formulae (ab initio RTA method), we were able to simulate the atomic data to compute the expansion opacity for Dy VIII. We have therefore shown that the RTA statistical method could be useful to overcome the difficulties encountered to obtain atomic data for very complex ions with usual atomic structure computational methods in order to estimate astrophysical opacities with a good level of reliability.

The results reported in the present work represent a significant contribution to one of the most important current hot topics in astrophysics, namely the analysis of the matter enriched with heavy elements ejected from neutron star mergers. The atomic data obtained in our study for moderately-charged lanthanide ions are certainly the most comprehensive and the most reliable available for assessing the opacities characterizing the early-phase kilonova spectra. Therefore, they constist in an important source of information for future astrophysical observations that will be made in this field of research. Indeed, with the upcoming new interferometers such as LIGO-India (LIGO-India collaboration, 2024) and Einstein telescope (Bureau de projet Einstein Telescope, 2024), very numerous atomic data as accurate as possible will be required to model kilonova spectra emitted after neutron star mergers which should be more and more commonly detected in the next few years, thereby providing a better understanding of how heavy trans-iron elements are produced in the Universe.

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Appendix A

Comparison of the radiative parameters for La V–X ions

Table A.1:	Transition	probabilities (g	A) and	d oscillator	strengths	(log(gf)) for	experimentally	observed
lines in La	V.							

λ_{obs} (Å) ^a	Т	ransition ^a	$qA (s^{-1})^b$	$\log(qf)^b$
000 ()	Lower level	Upper level	0 ()	0.007
389.034	$5s^25p^{5\ 2}P^o_{3/2}$	$5s^25p^46s(^1D_2, 1/2)_{3/2}$	3.25E+10	-0.14
390.722	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s(^1D_2, 1/2)_{5/2}$	4.38E+10	-0.05
398.531	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ (³ P)5d ² D _{3/2}	1.94E+09	-1.40
399.343	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s(^{3}P_1, 1/2)_{1/2}$	1.23E+09	-1.55
405.097	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s(^{3}P_1, 1/2)_{3/2}$	3.95E+10	-0.01
416.132	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s(^{3}P_0, 1/2)_{1/2}$	1.23E+09	-1.55
421.547	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^4(^{3}P)5d {}^{2}P_{1/2}$	1.23E+09	-1.55
423.074	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^4(^1S)5d\ ^2D_{5/2}$	3.03E+10	-0.13
424.784	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^46s(^1D_2, 1/2)_{3/2}$	2.71E+08	-2.15
432.108	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ (³ P)5d ² P _{3/2}	2.38E+11	0.76
435.275	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ (³ P)5d ² D _{5/2}	4.42E+11	1.02
436.135	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^4(^{3}P)5d ^{2}D_{3/2}$	3.07E+11	0.87
436.843	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^4(^1D)5d\ ^2S_{1/2}$	1.39E+11	0.51
437.107	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^46s(^{3}P_1, 1/2)_{1/2}$	1.16E+10	-0.50
437.551	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s(^{3}P_2, 1/2)_{3/2}$	2.00E+10	-0.27
444.010	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^46s(^{3}P_1, 1/2)_{3/2}$	5.57E+08	-1.78
444.067	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s(^{3}P_2, 1/2)_{5/2}$	6.87E+09	-0.75
450.405	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^4(^1S)5d\ ^2D_{3/2}$	2.00E+10	-0.27
457.303	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^46s(^{3}P_0, 1/2)_{1/2}$	6.73E+08	-1.71
463.848	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^4(^{3}P)5d {}^{2}P_{1/2}$	1.16E+10	-0.50
476.667	$5s^25p^5 {}^2P_{1/2}^{o}$	$5s^25p^4(^{3}P)5d ^{2}P_{3/2}$	5.57E+08	-1.71
482.164	$5s^25p^5 {}^2P_{3/2}^{o}$	$5s^25p^4(^1D)5d\ ^2F_{5/2}$	3.74E+09	-0.94
482.434	$5s^25p^5 {}^2P_{1/2}^{o}$	$5s^25p^4(^1D)5d\ ^2S_{1/2}$	6.75E+09	-0.72
483.298	$5s^25p^5 {}^2P_{1/2}^{o}$	$5s^25p^46s(^{3}P_2, 1/2)_{3/2}$	1.02E+10	-0.48
498.081	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ (³ P)5d ² F _{5/2}	1.85E+09	-1.22
499.028	$5s^25p^5 {}^2P_{1/2}^{o}$	$5s^25p^4(^1S)5d\ ^2D_{3/2}$	1.02E+10	-0.48
503.583	$5s^25p^5 {}^2P_{3/2}^{o'}$	$5s^25p^4(^1D)5d\ ^2D_{5/2}$	1.42E+09	-1.32
508.147	$5s^25p^5 {}^2P^{o'}_{3/2}$	$5s^25p^4(^1D)5d\ ^2P_{3/2}$	1.05E+07	-3.30
525.712	$5s^25p^5 {}^2P^{o'}_{3/2}$	$5s^25p^4(^1D)5d\ ^2D_{3/2}$	5.50E+08	-1.70
526.755	$5s^25p^5 {}^2P^{o'}_{3/2}$	$5s^25p^4(^3P)5d \ ^4P_{5/2}$	1.79E+09	-1.18
531.069	$5s^25p^5 {}^2P^{o'}_{3/2}$	$5s^25p^4(^3P)5d\ ^4F_{3/2}$	3.44E+09	-0.89
533.233	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^4(^3P)5d \ ^4F_{5/2}$	3.37E+09	-0.89
540.203	$5s^25p^5 {}^2P_{3/2}^{o'}$	$5s^25p^4(^1D)5d\ ^2P_{1/2}$	1.68E+09	-1.19
544.805	$5s^25p^5 {}^2P_{3/2}^{o'}$	$5s^25p^4(^3P)5d \ ^4P_{1/2}$	4.14E+08	-1.79
547.437	$5s^25p^5 {}^2P^{o'}_{3/2}$	$5s^25p^4(^3P)5d\ ^4P_{3/2}$	8.48E+08	-1.47
570.903	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^1D)5d\ ^2P_{3/2}$	1.06E+08	-2.35
593.181	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^1D)5d\ ^2D_{3/2}$	2.87E+08	-1.88
597.698	$5s^25p^5 {}^2P_{3/2}^{o'}$	$5s^25p^4(^{3}P)5d \ ^{4}D_{3/2}$	3.75E+07	-2.75
600.009	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^3P)5d\ ^4F_{3/2}$	1.67E+08	-2.11
600.237	$5s^25p^5 {}^2P_{3/2}^{o'}$	$5s^25p^4(^3P)5d\ ^4D_{5/2}$	1.15E+08	-2.26
611.695	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^1D)5d\ ^2P_{1/2}$	4.52E+07	-2.66
617.600	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^3P)5d\ ^4P_{1/2}$	1.05E+07	-3.29
620.981	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^3P)5d\ ^4P_{3/2}$	3.28E+07	-2.79
675.154	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^3P)5d\ ^4D_{1/2}$	1.76E+05	-5.00
686.469	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^4(^3P)5d\ ^4D_{3/2}$	2.56E+05	-4.70
699.449	$5s^25p^5 \ ^2P^{o'}_{3/2}$	$5s5p^{6}$ $^{2}S_{1/2}$	5.70E+08	-1.44
824.156	$5s^25p^5 \ ^2P_{1/2}^{o}$	$5s5p^{6} \ {}^{2}S_{1/2}$	3.53E+08	-1.52

^a Epstein and Reader (1976)

Table A.2: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in La VI.

$\lambda_{obs} (\text{\AA})^a$	Г	ransition ^a	$gA (s^{-1})^b$	$\log(gf)^{b}$
	Lower level	Upper level		
335.648	$5s^25p^4 {}^3P_1$	5s ² 5p ³ 6s 318315.7 ^o ₂	2.30E+10	-0.45
342.992	$5s^25p^{4} {}^1D_2$	$5s^25p^36s 320508.5^{o}_1$	2.69E+10	-0.36
343.921	$5s^25p^4 {}^3P_2$	$5s^25p^36s 290764.4^{\circ}_2$	1.05E+10	-0.77
345.202	$5s^25p^4 {}^3P_0$	$5s^25p^36s 302474.6^{o}_1$	2.54E+10	-0.39
345.589	$5s^25p^4 {}^1D_2$	$5s^25p^36s 318315.7^{\circ}_2$	3.02E+10	-0.31
347.338	$5s^25p^4 {}^3P_2$	$5s^25p^36s 287903.8^{\frac{1}{9}}_{2}$	7.08E+10	0.07
354.488	$5s^25p^4 {}^3P_1$	$5s^25p^36s 302474.6^{\circ}_1$	2.81E+09	-1.33
355.617	$5s^25p^4 {}^3P_2$	$5s^25p^36s 281198.0^{\circ}_{2}$	3.84E+10	-0.18
365.605	$5s^25p^{4-1}D_2$	$5s^25p^36s 302474.6^{\circ}_1$	8.30E+09	-0.83
369 847	$5s^{2}5n^{4}$ ³ P ₁	$5s^25n^36s$ 290764 4_0^o	1.02E+10	-0.72
370.037	$58^{2}5p^{4}{}^{3}P_{0}$	$5s^2 5p^3 6s 283029 4^{\circ}$	1.62E+10	-1.56
375 632	$5s^{2}5p^{4} {}^{3}P_{2}$	$5s^2 5p^3 6s 265029.1_1^{\circ}$	5.56E+10	0.03
380 739	$5s^{2}5p^{4}$ ³ P.	$5s^{2}5n^{3}6s^{2}830294^{o}$	$4.67E \pm 10$	-0.04
381.060	$5s^{2}5p^{4}$ ¹ D	$5s^{2}5p^{3}6s^{2}00764 4^{0}$	$1.06E \pm 11$	-0.04
383 173	$5s^{2}5p^{4}^{3}P$	$5s^{2}5p^{3}6s^{2}90704.4_{2}$	1.00E+11	0.52
202.425	$58 5p^{-1}F_1$	$5s^{2}5r^{3}6s^{2}201198.0_{2}$	1.13E+10	-0.04
201 127	$5s^{2}5p^{4}^{3}D$	$5s^{2}5p^{3}6s 520508.5_{1}^{2}$	4.31E+10	-0.07
384.427	$5s^{2}5p^{1}$ P_{2}	$5s^{2}5p^{2}6s 260127.8^{2}_{2}$	4.23E+09	-1.07
386.191	$5s^{2}5p^{1-1}D_{2}$	$5s^2 5p^8 6s 28/903.8^8_3$	9.93E+09	-0.70
387.591	$5s^2 5p^4 {}^{5}P_2$	$5s^2 5p^3 5d 258004.7_1^6$	1.63E+09	-1.4/
393.588	$5s^{2}5p^{4-1}D_{2}$	$5s^25p^36s\ 283029.4^{o}_1$	3.81E+09	-1.10
394.585	$5s^25p^4 {}^{3}P_0$	5s ² 5p ³ 6s 266218.0 ⁰ ₁	2.07E+10	-0.36
396.453	$5s^25p^4 {}^1D_2$	$5s^25p^36s\ 281198.0^o_2$	6.57E+09	-0.86
399.283	$5s^25p^4 {}^{3}P_2$	$5s^25p^35d 250443.6^o_2$	2.39E+09	-1.30
406.781	$5s^25p^4 {}^3P_1$	$5s^25p^36s \ 266218.0^o_1$	2.07E+10	-0.34
407.208	$5s^25p^4 \ ^3P_2$	$5s^25p^35d 245575.7^o_2$	4.27E+09	-0.96
407.799	$5s^25p^4 {}^3P_0$	$5s^25p^35d \ 258004.7^o_1$	1.29E+11	0.47
410.350	$5s^25p^4 \ ^3P_1$	5s ² 5p ³ 5d 264077.8 ₂ ^o	2.15E+11	0.17
412.210	$5s^25p^4 \ ^3P_2$	5s ² 5p ³ 5d 242595.3 ^o	6.62E+09	-0.89
412.210	$5s^25p^{4\ 1}S_0$	5s ² 5p ³ 6s 302474.6 ^o ₁	8.84E+09	-0.71
414.875	$5s^25p^4 \ ^3P_2$	5s ² 5p ³ 5d 241036.5 ^o ₃	4.38E+11	0.99
419.153	$5s^25p^4 {}^3P_0$	$5s^25p^35d 251363.6_1^o$	4.66E+10	0.05
419.226	$5s^25p^4 {}^3P_2$	$5s^25p^35d 238534.7^o_1$	8.98E+10	0.32
419.557	$5s^25p^4 {}^1D_2$	$5s^25p^35d 267303.0^{\circ}_3$	1.42E+09	-1.47
420.836	$5s^25p^4 {}^3P_1$	$5s^25p^35d 258004.7^{o}_1$	5.24E+10	0.07
422.414	$5s^25p^4 {}^3P_2$	$5s^25p^35d 236734.2^{\circ}_{23}$	7.40E+10	0.24
425.311	$5s^25p^{4} {}^1D_2$	$5s^25p^35d 264077.8^{\circ}_{\circ}$	5.59E+10	0.16
425.562	$5s^25p^4 {}^{3}P_1$	5s ² 5p ³ 5d 255365.8°	5.57E+10	0.10
428.291	$5s^25n^4$ ³ P ₂	$5s^25p^35d 233486.4^\circ$	2.46E+10	-0.21
430.356	$5s^25n^4 {}^{3}P_{2}$	$5s^25p^35d 232365 7^{\circ}$	8.58E+09	-0.66
430 761	$5s^25n^4$ ³ P ₂	$5s^2 5n^3 5d 232147 9^{\circ}$	7 50E+08	-1 70
432 940	$5s^{2}5p^{4}{}^{3}P_{2}$	$5s^{2}5n^{3}5d^{2}51363^{2}$	$5.24E \pm 10$	0.07
432.940	$5s^{2}5p^{4}^{3}P$	$5s^{2}5p^{3}5d^{2}504436^{0}$	3.24E+10 2.15E+11	0.07
434.007	$5s^{2}5p^{4}^{3}P$	$5s^{2}5p^{3}5d^{2}20445.02$	2.13E+11	0.72
433.141	$5s 3p F_0$ $5c^25r^4 1D$	5s 3p 3d 242393.31 $5c^25r^35d 259004.79$	4.00E+10	0.05
430.387	$5s 3p D_2$ $5a^25a^4 3D$	$5s^{2}5r^{3}5d^{2}28004.71$	0.36E+10	0.20
430.011	$5^{\circ}25^{-4}3^{\circ}$	$5s^{2}5n^{3}54^{2}45502.7^{2}_{2}$	2.10E+09	-1.1ð
444.060	$5s^{-}5p^{+}{}^{9}P_{1}$	$5s^{-}5p^{-}5d 2455/5.7_{2}^{0}$	1.00E+10	-0.50
444.839	$3s^{2}5p^{2}$ $^{4}1c^{2}$	$5s^{2}5p^{3}5d 224798.4^{0}_{1}$	1.06E+10	-0.55
448.136	$5s^{2}5p^{\pm 1}S_{0}$	5s ² 5p ³ 6s 283029.4 ⁰	3./9E+08	-2.00
449.627	$5s^{2}5p^{4} D_{2}$	$5s^25p^35d 251363.3^o_1$	2.46E+10	-0.20
450.020	$5s^{2}5p^{4} {}^{3}P_{1}$	5s ² 5p ³ 5d 242595.3 ^o	3.83E+10	-0.02
451.337	$5s^25p^4 {}^3P_2$	$5s^25p^35d 221564.0^o_2$	3.38E+09	-1.02
451.494	$5s^{2}5p^{4-1}D_{2}$	$5s^25p^35d 250443.6^{\circ}_{2}$	5.59E+10	0.16

Table	A.2:	Continue	ł.

λ_{obs} (Å) ^a	Т	Transition ^a	$gA(s^{-1})^b$	$\log(qf)^b$
	Lower level	Upper level	0	
461.640	$5s^25p^{4\ 1}D_2$	5s ² 5p ³ 5d 245575.7 ^o ₂	4.75E+09	-0.81
462.215	$5s^25p^4 {}^3P_1$	$5s^25p^35d 236734.2^{\circ}_2$	2.45E+06	-4.00
465.210	$5s^25p^4 {}^3P_2$	$5s^25p^35d 214956.5_1^{\circ}$	2.29E+08	-2.17
468.080	$5s^25p^4 {}^1D_2$	$5s^25p^35d 242595.3^{\circ}_1$	3.33E+10	-0.04
471.517	$5s^25p^4 {}^1D_2$	$5s^25p^35d 241036.5^{\circ}_3$	3.10E+08	-2.05
472.220	$5s^25p^4 {}^3P_1$	$5s^25p^35d 232147.9^3$	2.10E+09	-1.18
477.146	$5s^25p^4 {}^1D_2$	$5s^25p^35d 238534.7^{\frac{2}{0}}_{1}$	1.05E+10	-0.51
480.956	$5s^25p^4 {}^3P_1$	$5s^25p^35d 228302.7^{\circ}_2$	2.10E+09	-1.18
481.283	$5s^25p^4 {}^1D_2$	$5s^25p^35d 236734.2^{\frac{2}{9}}_{22}$	5.40E+09	-0.79
484.902	$5s^25p^4 {}^3P_2$	$5s^25p^35d \ 206227.2^{\circ}_3$	5.74E+09	-0.74
486.399	$5s^25p^4 {}^3P_1$	$5s^25p^35d 225975.1^9_0$	1.32E+09	-1.38
488.925	$5s^25p^4 {}^1D_2$	$5s^25p^35d 233486.4^{\circ}_3$	5.70E+09	-0.74
489.204	$5s^25p^4 {}^3P_1$	$5s^25p^35d 224798.4^{o}_1$	4.69E+09	-0.83
489.281	$5s^25p^4 {}^3P_2$	$5s^25p^35d 204381.5^{1}_{2}$	2.44E+09	-1.10
491.620	$5s^25p^{4} {}^1D_2$	$5s^25p^35d 232365.7^9_3$	5.91E+09	-0.71
492.146	$5s^25p^{4-1}D_2$	$5s^25p^35d 232147.9^{\circ}$	4.56E+07	-2.81
494.638	$5s^25p^4 {}^{3}P_0$	$5s^25p^35d 214956.5^{\circ}_1$	6.02E+09	-0.71
495.491	$5s^25p^4 {}^3P_2$	$5s^25p^35d \ 201819.9^{\circ}_{3}$	1.54E+09	-1.29
497.065	$5s^25p^4 {}^{3}P_1$	$5s^25p^35d 221564.0^\circ_2$	6.06E+08	-1.70
500.106	$5s^25p^4 {}^{3}P_2$	$5s^25p^35d$ 199957.4°	4.63E+08	-1.81
503.396	$5s^25p^4 {}^{3}P_2$	$5s^25p^35d$ 198650.7 ^o	1.76E+09	-1.22
504.738	$5s^25p^{4} {}^{1}S_0$	$5s^25p^35d 258004.7^{\circ}_1$	8.09E+08	-1.57
510.616	$5s^25p^4 {}^1D_2$	$5s^2 5p^3 5d 224798 4_1^0$	1 26E+09	-1.36
519.189	$5s^{2}5p^{4} {}^{1}D_{2}$	$5s^25p^35d 221564.0^\circ$	8.96E+08	-1.49
522.231	$5s^{2}5p^{4}$ ¹ S ₀	$5s^25p^35d 251363 3^{\circ}_{2}$	3 17E+08	-1.95
526.578	$5s^25p^4 {}^{3}P_{2}$	$5s^25p^35d$ 189905.4°	2.35E+09	-1.05
534 275	$5s^{2}5p^{4}{}^{3}P_{0}$	$5s^2 5p^3 5d 199957 4^o_1$	4 38E+08	-1 77
537.632	$5s^25p^{4} {}^1D_2$	$5s^25p^35d 214956.5^{\circ}_1$	8.15E+08	-1.51
539 480	$5s^{2}5p^{4} {}^{3}P_{2}$	5s5n ⁵ 185363 7 ^o	1 07E+09	-1 37
545.351	$5s^25p^4 {}^{3}P_{2}$	$5s^25p^35d$ 183366.3°	3.83E+08	-1.81
548.515	$5s^25p^4 {}^{3}P_{2}$	$5s^25p^35d$ 182310.1°	9.65E+08	-1.40
549 237	$5s^25n^4 {}^3P_2$	$5s^25n^35d$ 182070 9°	9.63E+08	-1 40
564 108	$5s^{2}5p^{4} {}^{1}D_{2}$	$5s^2 5p^3 5d 206227 2^{\circ}_{\circ}$	4 58E+08	-1 71
570.044	$5s^{2}5p^{4} {}^{1}D_{2}$	$5s^25p^35d 204381.5^\circ$	1.29E+08	-2.25
586 239	$5s^{2}5p^{4} {}^{3}P_{0}$	$5s^2 5p^3 5d 183366 3^{\circ}_{1}$	1.22E+08	-2.24
613.559	$5s^25p^4 {}^{3}P_1$	$5s^25p^35d$ 183366.3 ^o	2.93E+08	-1.83
615.372	$5s^25p^4 {}^{3}P_1$	$5s^25p^35d$ 182885.9°	2.40E+08	-1.92
621.313	$5s^25p^{4} {}^1D_2$	$5s^25p^35d$ 189905.4°	6.15E+07	-2.50
637.640	$5s^25p^4 {}^{3}P_2$	5s5p ⁵ 156828.3 ^o	1.49E+09	-1.08
639.357	$5s^25p^{4} {}^1D_2$	$585p^5$ 185363.7°	3.06E+09	-0.78
647.629	$5s^25p^{4} {}^1D_2$	$5s^25p^35d$ 183366.3°	6.48E+08	-1.44
652.092	$5s^25p^{4} {}^1D_2$	$5s^25p^35d$ 182310.1°	1.04E+07	-3.23
675.903	$5s^{2}5p^{4} {}^{3}P_{1}$	5s5p ⁵ 168332.8°	6.69E+08	-1.38
681.484	$5s^25n^4 {}^{3}P_{2}$	$5s5p^5$ 146738.0°	2.35E+09	-0.83
694,244	$5s^25p^4 {}^{3}P_{0}$	$5s5p^5$ 156828.3 ^o	6.28E+08	-1.39
732,891	$5s^25p^4 {}^{3}P_1$	$5s5p^5$ 156828.3 ^o	4.65E+08	-1.48
782.041	$5s^25n^{4}$ ¹ D ₂	5s5p ⁵ 156828.3 ^o	1.91E+08	-1.81
791.422	$5s^25p^4 {}^{3}P_1$	$5s5p^5$ 146738.0°	8.87E+08	-1.14
796.915	$5s^25p^{4}$	5s5p ⁵ 185363.7 ^o	2.34E+08	-1.72
849.028	$5s^25p^{4} {}^1D_2$	$5s5p^5$ 146738.0 ^o	3.79E+08	-1.45
1031.476	$5s^25p^{4} {}^{1}S_0^{2}$	5s5p ⁵ 156828.3 ^o ₁	3.43E+07	-2.34

^a Gayasov et al. (1997)

Table A.3:	Transition	probabilities (g	A) and	l oscillator	strengths	(log(gf))fd	or experimentally	observed
lines in La	VII.							

$\overline{\lambda_{obs}}$ (Å) ^a]	Fransition ^a	$\overline{gA} (\mathbf{s}^{-1})^b$	$\overline{\log(gf)}$
	Lower level	Upper level		
307.150	$5s^25p^3 \ ^2D^o_{3/2}$	$5s^25p^26s \ 345450.0_{5/2}$	3.23E+10	-0.37
308.473	$5s^25p^3 \ {}^4S^o_{3/2}$	5s ² 5p ² 6s 324181.0 _{3/2}	7.91E+09	-0.98
310.991	$5s^25p^3 \ ^2D_{5/2}^{o}$	5s ² 5p ² 6s 348538.0 _{3/2}	1.92E+10	-0.59
311.627	$5s^25p^3 \ {}^4S^o_{3/2}$	5s ² 5p ² 6s 320896.3 _{5/2}	6.53E+10	-0.05
313.553	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s^25p^26s$ 318923.0 _{1/2}	5.56E+09	-1.12
314.007	$5s^25p^3 {}^2D_{5/2}^{o}$	$5s^25p^26s$ 345450.0 _{5/2}	5.98E+10	-0.08
318.237	$5s^25p^3 \ {}^4S^{o}_{3/2}$	5s ² 5p ² 6s 314222.0 _{3/2}	2.45E+10	-0.46
328.609	$5s^25p^3 {}^2D_{3/2}^{o}$	5s ² 5p ² 6s 324181.0 _{3/2}	1.77E+10	-0.58
334.395	$5s^25p^3 {}^2D^o_{3/2}$	$5s^25p^26s \ 318923.0_{1/2}$	4.77E+10	-0.13
336.491	$5s^25p^3 {}^2D^o_{5/2}$	$5s^25p^26s 324181.0_{5/2}$	7.32E+10	0.06
337.143	$5s^25p^3 \ ^4S^o_{2/2}$	$5s^25p^26s 296609.8_{1/2}$	2.08E+10	-0.48
339.738	$5s^25p^3 {}^2D_{2/2}^{o}$	$5s^25p^26s 314222.0_{3/2}$	3.75E+09	-1.22
340.255	$5s^25p^3 {}^2D_{r/2}^{o}$	$5s^25p^26s$ 320896.35/2	2.45E+10	-0.40
343.848	$5s^25p^3 {}^2P_{o}^{o}$	$5s^25p^26s 348538.0_{3/2}$	7.20E+10	0.07
347 540	$5s^25n^{3}{}^{2}P^{o}$	$5s^2 5n^2 6s 345450 0r / 2$	1 87E+10	-0.51
348 164	$5s^{2}5n^{3}{}^{2}D^{o}$	$5s^{2}5p^{2}6s^{3}14222 0_{a/a}$	7.11E+09	-0.92
352 745	$5s^{2}5p^{3}^{2}D_{5/2}^{0}$	$5s^{2}5p^{2}6s^{3}241810_{s}$	$3.66E \pm 10$	0.92
350 / 10	$5s 5p 1_{1/2}$ $5s^2 5p^3 2p^o$	$5s^{2}5p^{2}6s^{2}180230$	$1.88E \pm 10$	0.20
279 022	$5s 5p 1_{1/2}$ $5s^2 5p^3 2D^o$	$5s^{2}5p^{2}5d^{2}008007$	6 09E 10	1.96
270.040	$5s \ 5p \ D_{5/2}$	$5s \ 5p \ 5u \ 290890.7_{5/2}$	$0.90E \pm 00$	-1.60
200 529	$5s^{-}5p^{-}+P_{3/2}^{-}$	$5s^{-}5p^{-}0s^{-}520890.5_{5/2}$	1.01E+09	-1.50
390.528	$5s^{-}5p^{-}1S_{3/2}^{-}$	$5s^{2}5p^{2}5d$ 256064.4 _{5/2}	5.82E+10	-0.11
397.462	$5s^25p^{3-4}S_{3/2}^{6}$	$5s^2 5p^2 5d 251595./_{3/2}$	5.3/E+10	0.07
401.619	$5s^25p^{3/2}P_{1/2}^{5/2}$	$5s^25p^25d 289686.6_{3/2}$	7.59E+10	0.22
403.228	$5s^25p^3 {}^2D_{5/2}^o$	$5s^25p^25d 274989.8_{5/2}$	1.68E+10	-0.40
407.895	$5s^25p^3 {}^2D_{5/2}^o$	5s ² 5p ² 5d 272152.3 _{7/2}	2.71E+11	0.77
408.263	$5s^25p^3 {}^4S^o_{3/2}$	$5s^25p^25d 244939.9_{1/2}$	9.46E+10	0.32
410.550	$5s^25p^3 {}^4S^o_{3/2}$	$5s^25p^25d 243575.9_{3/2}$	1.08E+11	0.39
411.113	$5s^25p^3 \ ^2D^o_{3/2}$	$5s^25p^25d \ 263111.5_{5/2}$	4.66E+10	0.01
412.045	$5s^25p^3 \ ^2D^o_{3/2}$	$5s^25p^25d \ 262560.6_{3/2}$	1.01E+10	-0.68
412.389	$5s^25p^3 \ ^2D^o_{3/2}$	$5s^25p^25d \ 262358.0_{1/2}$	5.98E+08	-1.86
414.949	$5s^25p^3 \ {}^4S^o_{3/2}$	5s ² 5p ² 5d 240993.5 _{5/2}	2.33E+11	0.73
420.550	$5s^25p^3 \ {}^4S^o_{3/2}$	5s5p ⁴ 237784.9 _{3/2}	4.88E+09	-0.86
421.545	$5s^25p^3 \ ^2D_{3/2}^{o}$	5s5p ⁴ 257090.8 _{1/2}	5.69E+10	0.13
423.376	$5s^25p^3 {}^2D_{3/2}^{o'}$	$5s^25p^25d \ 256064.4_{5/2}$	6.73E+10	0.20
423.511	$5s^25p^3 {}^2D_{5/2}^o$	$5s^25p^25d \ 263111.5_{5/2}$	6.98E+10	0.20
424.503	$5s^25p^3 {}^2D_{5/2}^{o}$	$5s^25p^25d \ 262560.6_{3/2}$	9.38E+07	-2.69
428.858	$5s^25p^3 {}^2P^o_{3/2}$	$5s^25p^25d 290890.7_{5/2}$	1.22E+11	0.48
431.082	$5s^25p^3 {}^2P_{3/2}^{o}$	$5s^25p^25d 289686.6_{3/2}$	2.08E+10	-0.28
436.537	$5s^25p^3 {}^2D_{r/2}^{o}$	$5s^25p^25d 256064.4_{5/2}$	9.41E+10	0.38
438.915	$5s^25p^3 {}^{4}S_{2/2}^{o}$	$5s^25p^25d 227834.4_{5/2}$	1.11E+10	-0.52
445.236	$5s^25p^3 {}^2D_{e}^o$	$5s^25p^25d 251595.7_{3/2}$	1.35E+10	-0.44
447 006	$5s^25n^3 {}^2D_{5/2}^o$	$5s^2 5n^2 5d 243575 9_{3/2}$	1.61E+10	-0.37
450 479	$5s^{2}5n^{3} 4S^{o}$	$5s^{2}5p^{2}5d^{2}21987^{2}9a^{2}$	4 88F+09	-0.86
450 727	$5s^25n^3 {}^2\mathbf{P}^o$	$5s^25n^25d$ 262560 6	3 97F±10	-0.03
451 140	$5s^{2}5n^{3}{}^{2}D^{0}$	$5s^25n^25d$ 262200.03/2	5.72LT10	0.05
452 222	$5s \ 3p \ r_{1/2}$ $5s^2 5n^3 \ ^2 D^o$	$5s^25n^254 240002 5$	$1.71E \cdot 10$	0.14
+52.233	$5^{5} J^{2} J^{2$	$5s^{2}5n^{2}5d^{2}404995.55/2$	1.71E+10	-0.33
434.303	$5s \ 5p^2 - D_{5/2}^2$	$5s \text{ sp su } 24/011.8_{7/2}$	0.23E+09	-0.74
438.894	$5s^{-}5p^{-3}D_{3/2}^{-3}$	$5s3p^{-} 257/84.9_{3/2}$	4.41E+10	0.09
401./12	$5s^{-}5p^{\circ} D_{5/2}^{\circ}$	58-5p-5d 243575.9 _{3/2}	2.91E+10	-0.08
462.119	$5s^2 5p^3 {}^2 P_{1/2}^0$	$585p^{-1}25/090.8_{1/2}$	8.04E+09	-0.65
464.837	$5s^{2}5p^{3} {}^{4}S^{o}_{3/2}$	5s ² 5p ² 5d 215130.0 _{5/2}	2.87E+09	-1.06
467.283	$5s^25p^3 {}^2D_{5/2}^o$	5s ² 5p ² 5d 240993.5 _{5/2}	1.54E+10	-0.35

Table A.3: Continued.

λ_{obs} (Å) ^a	Г	Transition ^a	$gA (s^{-1})^b$	$\log(gf)^b$
	Lower level	Upper level		
469.949	$5s^25p^3 {}^2D^o_{5/2}$	$5s^25p^25d 239780.2_{7/2}$	1.12E+10	-0.46
474.158	$5s^25p^3 {}^2P_{1/2}^{o}$	5s ² 5p ² 5d 251595.7 _{3/2}	5.40E+09	-0.79
474.395	$5s^25p^3 {}^2D^o_{5/2}$	5s5p ⁴ 237784.9 _{3/2}	5.10E+09	-0.62
480.843	$5s^25p^3 {}^2D_{3/2}^{o}$	$5s^25p^25d 227834.4_{5/2}$	3.83E+09	-0.91
483.627	$5s^25p^3 {}^2D_{3/2}^{o}$	$5s^25p^25d 226638.4_{1/2}$	2.27E+09	-1.12
485.238	$5s^25p^3 {}^4S^{o'}_{3/2}$	$5s^25p^25d \ 206084.9_{5/2}$	6.98E+09	-0.64
494.638	$5s^25p^3 {}^4S^{o}_{3/2}$	5s ² 5p ² 5d 202171.9 _{3/2}	2.18E+09	-1.13
494.751	$5s^25p^3 {}^2D_{3/2}^{o}$	$5s^25p^25d 221987.9_{3/2}$	9.14E+08	-1.51
497.901	$5s^25p^3 {}^2D_{5/2}^{o'}$	$5s^25p^25d$ 227834.4 _{5/2}	3.88E+09	-0.87
500.106	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s5p^4$ 199957.0 _{1/2}	1.09E+09	-1.42
501.559	$5s^25p^3 {}^2P^{o'}_{3/2}$	$5s5p^4$ 257090.8 _{1/2}	7.52E+09	-0.61
504.210	$5s^25p^3 {}^2D^o_{3/2}$	$5s^25p^25d \ 218195.0_{1/2}$	6.91E+08	-1.61
505.704	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s^25p^25d$ 197741.4 _{3/2}	2.41E+08	-2.06
512.826	$5s^25p^3 {}^2D_{5/2}^{o}$	$5s^25p^25d \ 221987.9_{3/2}$	5.15E+09	-0.72
531.518	$5s^25p^3 {}^2D_{5/2}^{o'}$	$5s^25p^25d \ 215130.0_{5/2}$	1.22E+08	-2.32
537.007	$5s^25p^3 {}^2D_{3/2}^{o'}$	$5s^25p^25d \ 206084.9_{5/2}$	2.78E+08	-1.95
545.705	$5s^25p^3 {}^4S^{o}_{3/2}$	5s5p ⁴ 183252.2 _{5/2}	7.62E+07	-2.49
548.514	$5s^25p^3 {}^2D^o_{3/2}$	5s ² 5p ² 5d 202171.9 _{3/2}	1.51E+09	-1.20
551.608	$5s^25p^3 {}^2P_{1/2}^{o'}$	$5s^25p^25d 221987.9_{3/2}$	2.37E+08	-2.00
555.264	$5s^25p^3 {}^2D_{3/2}^{o}$	5s5p ⁴ 199957.0 _{1/2}	4.90E+09	-0.68
558.366	$5s^25p^3 {}^2D_{5/2}^{o}$	$5s^25p^25d \ 206084.9_{5/2}$	4.42E+08	-1.72
562.201	$5s^25p^3 {}^2D_{3/2}^{o}$	5s ² 5p ² 5d 197741.4 _{3/2}	1.50E+08	-2.18
563.387	$5s^25p^3 {}^2P_{1/2}^{o/2}$	$5s^25p^25d \ 218195.0_{1/2}$	6.45E+08	-1.54
565.820	$5s^25p^3 \ {}^{4}S^{o}_{3/2}$	5s5p ⁴ 176734.1 _{3/2}	5.54E+08	-1.60
570.840	$5s^25p^3 {}^2D_{5/2}^o$	$5s^25p^25d 202171.9_{3/2}$	4.59E+09	-0.68
585.655	$5s^25p^3 {}^2D_{5/2}^{o}$	5s ² 5p ² 5d 197741.4 _{3/2}	5.10E+09	-0.62
591.969	$5s^25p^3 {}^2P^o_{3/2}$	$5s^25p^25d 226638.4_{1/2}$	3.54E+09	-0.77
608.732	$5s^25p^3 {}^2P^{o}_{3/2}$	5s ² 5p ² 5d 221987.9 _{3/2}	2.29E+08	-1.94
612.043	$5s^25p^3 {}^2D^o_{3/2}$	5s5p ⁴ 183252.2 _{5/2}	1.34E+07	-3.15
619.281	$5s^25p^3 {}^2P_{1/2}^{o/2}$	5s ² 5p ² 5d 202171.9 _{3/2}	5.20E+07	-2.56
623.136	$5s^25p^3 {}^2P_{3/2}^{o}$	$5s^25p^25d \ 218195.0_{1/2}$	6.20E+08	-1.49
623.935	$5s^25p^3 \ {}^4S^o_{3/2}$	5s5p ⁴ 160273.2 _{1/2}	1.68E+09	-1.03
627.906	$5s^25p^3 {}^2P_{1/2}^{o}$	5s5p ⁴ 199957.0 _{1/2}	2.26E+09	-0.92
636.341	$5s^25p^3 {}^4S^{o}_{3/2}$	5s5p ⁴ 157148.5 _{3/2}	3.32E+09	-0.71
636.763	$5s^25p^3 {}^2P_{1/2}^{o}$	$5s^25p^25d$ 197741.4 _{3/2}	8.73E+08	-1.31
637.490	$5s^25p^3 {}^2D_{3/2}^{o}$	5s5p ⁴ 176734.1 _{3/2}	5.57E+09	-0.50
639.956	$5s^25p^3 {}^2D_{5/2}^{o}$	5s5p ⁴ 183252.2 _{5/2}	5.63E+09	-0.48
667.813	$5s^25p^3 {}^2D_{5/2}^{o}$	$5s5p^4$ 176734.1 _{3/2}	2.41E+08	-1.82
692.227	$5s^25p^3 {}^2P^{o}_{3/2}$	$5s^25p^25d 202171.9_{3/2}$	3.01E+08	-1.71
697.596	$5s^25p^3 {}^{4}S^{o}_{3/2}$	5s5p ⁴ 143349.5 _{5/2}	2.77E+09	-0.72
703.005	$5s^25p^3 {}^2P^o_{3/2}$	$5s5p^4$ 199957.0 _{1/2}	1.26E+08	-2.08
712.219	$5s^25p^3 {}^2D_{2/2}^o$	$5s5p^4$ 160273.2 _{1/2}	7.97E+07	-2.24
728.439	$5s^25p^3 {}^2D_{2/2}^{o}$	$5s5p^4$ 157148.5 _{3/2}	1.16E+06	-4.05
735.096	$5s^25p^3 {}^2P_{1/2}^{o}$	$5s5p^4$ 176734.1 _{3/2}	2.31E+08	-1.76
768.302	$5s^25p^3 {}^2D_{r/2}^{o}$	5s5p ⁴ 157148.5 _{3/2}	1.79E+08	-1.83
796.540	$5s^25p^3 {}^2P_{2/2}^o$	5s5p ⁴ 183252.2 _{5/2}	1.55E+09	-0.87
809.841	$5s^25p^3 {}^2D_{a/c}^{o}$	5s5p ⁴ 143349.5 _{5/2}	7.04E+08	-1.19
836.288	$5s^25p^3 {}^2P_{1/2}^{o}$	$5s5p^4$ 160273.2 _{1/2}	1.28E+08	-1.90
859.416	$5s^25p^3 {}^2D_{r/2}^{o}$	5s5p ⁴ 143349.5 _{5/2}	3.47E+08	-1.44
975.027	$5s^25p^3 {}^2P_{a/a}^{o}$	5s5p ⁴ 160273.2 _{1/2}	1.32E+07	-2.77
1005.649	$5s^25p^3 {}^2P^{o}_{3/2}$	5s5p ⁴ 157148.5 _{3/2}	7.44E+07	-1.99

^a Gayasov et al. (1998)

) ())				
$\lambda_{obs} (A)^a$	Tra	ansition ^a	$gA (s^{-1})^b$	$\log(gf)^b$
	Lower level	Upper level		
280.260	$5s^25p^2 \ ^3P_1$	5s ² 5p6s ³ P ₂ ^o	2.80E+10	-0.50
284.336	$5s^25p^2 \ ^3P_0$	5s ² 5p6s ³ P ₁ ^o	3.28E+10	-0.41
285.384	$5s^25p^2 \ ^3P_2$	5s ² 5p6s ³ P ₂ ^o	4.72E+10	-0.26
302.277	$5s^25p^2 \ ^3P_1$	5s ² 5p6s ³ P ₀ ^o	2.55E+10	-0.47
303.414	$5s^25p^2 \ ^1D_2$	$5s^25p6s \ ^1P_1^o$	7.85E+10	0.01
306.767	$5s^25p^2 \ ^3P_2$	5s ² 5p6s ³ P ₁ ^o	5.57E+10	-0.12
307.321	$5s^25p^2 \ ^1D_2$	5s ² 5p6s ³ P ₂ ^o	3.07E+10	-0.39
322.811	$5s^25p^2 \ ^1S_0$	$5s^25p6s \ ^1P_1^o$	1.48E+10	-0.66
370.024	$5s^25p^2 \ ^3P_0$	5s ² 5p5d 270253 ^o ₁	4.21E+08	-2.10
379.061	$5s^25p^2 \ ^3P_2$	5s ² 5p5d 289537 ^o ₃	2.00E+10	-0.41
391.082	$5s^25p^2 \ ^3P_1$	$5s^25p5d 275025_1^o$	4.34E+09	-1.11
395.969	$5s^25p^2 \ ^3P_1$	5s ² 5p5d 271866 ^o ₀	2.89E+10	-0.20
398.509	$5s^25p^2 \ ^3P_1$	$5s^25p5d 270253_1^o$	5.09E+10	0.04
400.709	$5s^25p^2 \ ^3P_1$	$5s^25p5d \ 268878^o_2$	1.66E+10	-0.44
401.128	$5s^25p^2 \ ^3P_2$	$5s^25p5d 275025^{\overline{o}}_1$	1.71E+10	-0.41
401.290	$5s^25p^2 \ ^3P_0$	5s ² 5p5d 249196 ^o ₁	3.75E+10	-0.07
401.373	$5s^25p^2 \ ^3P_2$	$5s^25p5d 274872^o_2$	4.19E+10	-0.02
407.895	$5s^25p^2 \ ^3P_2$	$5s^25p5d 270890^{\overline{o}}_3$	1.81E+11	0.62
408.095	$5s^25p^2 {}^3P_0$	$5s^25p5d 245042_1^{\circ}$	7.93E+09	-0.73
408.959	$5s^25p^2 \ ^3P_2$	5s ² 5p5d 270253 ^o ₁	3.37E+09	-1.08
411.267	$5s^25p^2 \ ^3P_2$	$5s^25p5d \ 268878^o_2$	5.11E+07	-2.82
418.762	$5s^25p^2 \ ^1D_2$	$5s^25p5d \ 289537_3^{\overline{o}}$	4.92E+10	0.05
435.017	$5s^25p^2 \ ^3P_1$	5s ² 5p5d 249196 ^o ₁	1.46E+10	-0.42
438.465	$5s^25p^2 \ ^3P_1$	$5s^25p5d 247389^o_2$	5.52E+10	0.17
443.030	$5s^25p^2 {}^3P_1$	$5s5p^3 245042_1^o$	1.02E+10	-0.56
445.851	$5s^25p^2 {}^1D_2$	$5s^25p5d 275025_1^o$	1.41E+10	-0.41
446.161	$5s^25p^2 \ ^1D_2$	$5s^25p5d 274872^{o}_2$	2.64E+10	-0.14
451.140	$5s^25p^2 {}^3P_2$	$5s^25p5d 247389^{o}_2$	1.67E+10	-0.33
454.230	$5s^25p^2 {}^1D_2$	$5s^25p5d 270890^{\circ}_3$	2.31E+10	-0.19
455.551	$5s^25p^2 {}^1D_2$	$5s^25p5d 270253_1^{\circ}$	1.88E+09	-1.38
455.956	$5s^25p^2 {}^3P_2$	$5s5p^3 245042_1^{o}$	5.18E+08	-1.83
458.423	$5s^25p^2 {}^1D_2$	$5s^25p5d 268878^o_2$	3.17E+10	-0.04
459.727	$5s^25p^2 {}^3P_0$	$5s5p^{3} 217519_{1}^{o}$	1.12E+10	-0.49
466.767	$5s^25p^2 {}^3P_2$	$5s^{2}5p5d 239969^{o}_{3}$	2.94E+09	-1.00
477.454	$5s^25p^2 {}^3P_1$	$5s^25p5d 228766^o_2$	2.02E+09	-1.18
479.129	$5s^25p^2 {}^3P_2$	$5s5p^24f 234437_3^{\circ}$	1.35E+10	-0.37
489.046	$5s^25p^2 {}^1S_0$	$5s^{2}5p5d 275025_{1}^{o}$	6.04E+07	-2.70
492.517	$5s^25p^2 {}^3P_2$	$5s^25p5d 228766^{o}_2$	3.99E+09	-0.86
503.887	$5s^25p^2 {}^1D_2$	$5s^25p5d 249196_1^2$	7.25E+09	-0.60
504.545	$5s^25p^2 {}^3P_1$	$5s^25p5d 217519_1^{\circ}$	1.93E+10	-0.18
507.156	$5s^25p^2 {}^3P_1$	$5s5p^3 216497^{\circ}_{2}$	4.24E+08	-1.79
508.511	$5s^25p^2 {}^1D_2$	5s ² 5p5d 247389 ^o	3.40E+09	-0.92

Table A.4: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in La VIII.

Table A.4: Continued.

λ_{obs} (Å) ^a	Tra	ansition ^a	$gA (s^{-1})^b$	$\log (qf)^b$
	Lower level	Upper level	0	0
511.630	$5s^25p^2 {}^3P_0$	5s5p ³ 195453 ^o ₁	1.95E+09	-1.12
514.659	$5s^25p^2 {}^1D_2$	$5s5p^3 245042_1^{o}$	2.68E+10	-0.02
521.397	$5s^25p^2 \ ^3P_2$	$5s5p^3 217519^{o}_1$	4.70E+10	0.24
528.453	$5s^25p^2 \ ^1D_2$	5s ² 5p5d 239969 ^o ₃	1.05E+08	-2.38
544.375	$5s^25p^2 \ ^1D_2$	5s5p ² 4f 234437 ^o ₃	1.05E+08	-2.38
559.753	$5s^25p^2 \ ^1S_0$	5s ² 5p5d 249196 ^o ₁	2.03E+08	-2.07
561.708	$5s^25p^2 \ ^1D_2$	$5s^25p5d 228766_2^o$	2.03E+09	-1.04
567.753	$5s^25p^2 \ ^3P_1$	$5s5p^3$ 195453 ^o ₁	6.55E+09	-0.51
573.071	$5s^25p^2 \ ^1S_0$	$5s5p^3 245042_1^o$	4.18E+09	-0.73
575.852	$5s^25p^2 \ ^3P_1$	$5s5p^3$ 192976 ^o ₀	2.29E+09	-0.96
584.760	$5s^25p^2 \ ^3P_2$	$5s5p^3$ 196738 $_2^o$	1.22E+10	-0.21
589.188	$5s^25p^2 \ ^3P_2$	$5s5p^3$ 195453 ^o ₁	2.58E+08	-1.88
599.598	$5s^25p^2 \ ^1D_2$	5s5p ³ 217519 ^o ₁	7.18E+08	-1.47
603.291	$5s^25p^2 \ ^1D_2$	$5s5p^3 216497^o_2$	1.04E+10	-0.26
603.881	$5s^25p^2 \ ^3P_0$	$5s5p^3$ 165594 $_1^o$	4.17E+09	-0.64
664.918	$5s^25p^2 \ ^3P_2$	5s5p ³ 176121 ^o ₃	3.31E+09	-0.66
669.155	$5s^25p^2 \ ^3P_1$	$5s5p^3$ 168764 $_2^o$	4.42E+09	-0.53
680.391	$5s^25p^2 {}^1S_0$	$5s5p^3 217519_1^o$	7.22E+08	-1.36
684.932	$5s^25p^2 \ ^1D_2$	$5s5p^3$ 196738 $_2^o$	4.00E+08	-1.57
699.114	$5s^25p^2 \ ^3P_2$	$5s5p^3$ 168764 $_2^o$	5.05E+07	-2.43
714.960	$5s^25p^2 \ ^3P_2$	$5s5p^3$ 165594 $_1^o$	3.36E+08	-1.60
797.561	$5s^25p^2 \ ^1D_2$	5s5p ³ 176121 ^o ₃	1.84E+09	-0.76
800.581	$5s^25p^2 {}^1S_0$	$5s5p^3$ 195453 ^o ₁	1.79E+08	-1.78
842.378	$5s^25p^2 \ ^3P_1$	$5s5p^3 \ 138032^o_2$	2.34E+08	-1.60
847.275	$5s^25p^2 \ ^1D_2$	$5s5p^3$ 168764 $_2^o$	7.66E+07	-2.10
870.654	$5s^25p^2 \ ^1D_2$	5s5p ³ 165594 ^o ₁	1.21E+08	-1.88
890.432	$5s^25p^2 \ ^3P_2$	$5s5p^3 \ 138032_2^o$	1.77E+08	-1.67
1052.091	$5s^25p^2 \ ^1S_0$	$5s5p^3$ 165594 $_1^o$	1.53E+07	-2.62
1145.559	$5s^25p^2 \ ^1D_2$	$5s5p^3 \ 138032_2^o$	1.45E+07	-2.55

^a Tauheed et al. (2008)

Table A.5:	Transition	probabilities (gA) and	d oscillator	strengths	(log(gf))fd	or experimentally	v observed
lines in La	IX.							

$(\mathring{A})a$	Tron	vition	~ 4	(a-1)	log(af)
Λ_{obs} (A)	I awar laval	Unner level	<i>gA</i>	(S) This work ^c	$\log(g_f)$
202 202	5 -24 f 2 D 0	5 2 5 x 502 8 50	Plevious		
202.393	$58^{-}41^{-}F_{5/2}^{-}$	58-58 595859 _{7/2}		2.03E+11	0.19
202.824	$5s^24f^2F_{7/2}^6$	5s ² 5g 594699 _{9/2}		3.19E+11	0.28
262.285	$5s^25p\ ^2P^o_{1/2}$	$5s^26s \ 381269.3_{1/2}$		4.05E+10	-0.39
283.280	$5s^25p\ ^2P^o_{3/2}$	5s ² 6s 381269.3 _{1/2}		6.60E+10	-0.12
340.368	$5s^25p\ ^2P_{1/2}^{o'}$	5s5p4f 293802.3 _{3/2}		2.24E+10	-0.43
363.478	5s5p ² 127670.4 _{1/2}	$4f5p^2 402790^o_{3/2}$	1.20E+10	2.31E+09	-1.32
368.754	$5s^25p ^2P_{1/2}^o$	5s5p4f 271182.1 _{3/2}		4.59E+10	-0.03
372.062	$5s^25p P_{3/2}^{0}$	5s5p4f 297037.65/2		3.77E+10	-0.13
372 247	$5s5n^2$ 153628 1 _{5/2}	5s5n5d 422273°	2 60E+10	1.60E+10	-0.50
373 572	$5s5p^2$ 174450 3-12	5s5p5d 422275 _{7/2}	2.60E+11	1.66E+11	0.50
274.074	$5s5p^{-174459.53/2}$	$5s_{5/2}^{26}$	2.00E+11	4.75E+00	1.02
374.074	585p 174459.5 _{3/2}	$58 \text{ op } 441779_{1/2}$	7.00E+09	4.73E+09	-1.05
3/5.118	$5s5p^2$ 191315. $3_{1/2}$	$555p5d 45/898_{1/2}^{\circ}$	3.00E+10	3.31E+10	-0.18
377.367	$5s5p^2$ 184888.4 _{5/2}	5s5p5d 449886 $_{7/2}^{o}$	2.24E+11	6.08E+10	0.11
377.367	5s5p ² 143356.9 _{3/2}	5s5p5d 408346 _{3/2}	8.10E+10	2.55E+10	-0.26
377.717	5s5p ² 143356.9 _{3/2}	5s5p5d 408104 $^o_{5/2}$	7.80E+10	5.34E+10	0.04
378.157	5s5p ² 143356.9 _{3/2}	$4f5p^2 407797^o_{1/2}$	4.20E+10	1.19E+10	-0.61
382.215	5s5p ² 143356.9 _{3/2}	$5s5p5d 404990_{1/2}^{o}$	2.40E+10	4.77E+10	0.01
382.303	$5s5p^2$ 143356.9 _{3/2}	$4f5p^2 404935_{0}^{a}$	6.00E+09	3.86E+09	-1.09
384,691	$5s5p^2$ 127670 41/2	5s5n5d 387619°	9.20E+10	7.78E+10	0.23
385 051	$5s5n^2$ 127670 4	$5s5n5d 386770^{\circ}$	$1.12E_{11}$	1.02E+10	0.35
201 044	$5_{0}5_{p}^{2}$ 152620 1	$45n^2 408760^0$	2.20E + 10	8 17E . 00	0.75
391.940	5.5.2 153028.1 _{5/2}	413p 408/09 _{7/2}	5.20E+10	0.1/E+U9	-0.75
392.590	$5s5p^2$ 153628.1 _{5/2}	$5s5p5d 408346_{3/2}^{\circ}$	3.20E+10	1.96E+10	-0.34
392.960	$5s5p^2$ 153628.1 _{5/2}	5s5p5d 408104 $^o_{5/2}$	1.24E+11	9.45E+10	0.32
393.098	5s5p ² 153628.1 _{5/2}	5s5p5d 408018° _{7/2}	2.34E+11	1.92E+11	0.63
394.802	$5s5p^2$ 184888.4 _{5/2}	5s5p5d 438182 _{7/2}	1.06E+11	6.08E+10	0.11
395.074	$5s^25p\ ^2P_{1/2}^o$	5s ² 5d 253117.3 _{3/2}		8.37E+09	-0.69
395.557	5s5p4f 247782 _{5/2}	5s ² 5f 500588 ^o _{7/2}	2.90E+10	1.18E+10	-0.60
399.607	$5s5p^2$ 191315.31/2	5s5p5d 441561°	2.80E+10	3.31E+10	-0.18
399.867	$5s^25d$ 249703 $5z/2$	$5s^25f 499784c^{0}$	1.02E+11	1.14E+11	0.41
400 478	$5s^25n^2P^0$.	$5s5n4f 249703 5_{0.00}$		4 59F+10	0.03
400.470	$5_{8}5_{p}^{2} 1_{1/2}^{1/2}$	$4f5n^2$ 302088°	7 00E±09	5 10E+00	0.03
400.399	$5_{3}5_{p}^{2} = 143350.93/2$	$415p^{-}592900_{3/2}$	7.00E+09	1.59E+10	-0.95
402.560	585p 145550.9 _{3/2}	415p 591878 _{5/2}	2.00E+10	1.36E+10	-0.44
402.961	$5s5p^2 12/6/0.4_{1/2}$	$5p^{\circ} 3/5835_{3/2}^{\circ}$	7.00E+09	7.54E+09	-0.75
404.216	5s5p ² 153628.1 _{5/2}	$415p^2 401024_{5/2}^6$	2.20E+10	3.51E+10	-0.08
405.407	5s5p4f 253117.3 _{3/2}	$5s^25f 499784^o_{5/2}$	6.90E+10	2.18E+10	-0.33
405.654	5s5p4f 254070.0 _{5/2}	$5s^25f \ 500588^o_{7/2}$	1.02E+11	2.42E+11	0.78
406.546	5s5p ² 174459.3 _{3/2}	4f5p ² 420432 ^o _{5/2}	1.50E+10	9.99E+08	-1.60
406.819	5s5p ² 191315.3 _{1/2}	5s5p5d 437125°	1.13E+11	7.89E+10	0.29
409.397	5s5p ² 143356.9 _{3/2}	5s5p5d 387619°	2.00E+09	1.63E+09	-1.40
410.820	$5s5p^2$ 143356.9 _{2/2}	$5s5p5d 386770^{o}_{2}$	2.50E+10	2.21E+10	-0.27
411 272	$585n^2$ 221736 4	$4f5n^2 464884^o$	1.31E+11	2.48E+09	-1.19
411 363	$5e5n^2$ 153628 1.	4f5n ² 3067240	$4.10E \pm 10$	5.55E+10	0.13
411 670	$5s^25p$ $10020.15/2$	$-15p$ 59072 $+_{7/2}$	7.10ET10	1 15E 10	0.15
412.502	$55 \text{ Sp } \mathbf{r}_{3/2}$	555754 41 (2000)	5 00E 10	1.13E+10	-0.55
412.502	555p ⁻ 1/4459.3 _{3/2}	585p5a 416886 _{3/2}	5.20E+10	4.54E+10	0.04
413.257	5s5p ² 221/36.4 _{3/2}	5s5p5d 463/17 ^o _{3/2}	1.21E+11	1.55E+07	-3.40
414.094	5s5p ² 221736.4 _{3/2}	$415p^2 \ 463230^o_{5/2}$	1.40E+11	1.88E+11	0.67
415.112	5s5p ² 143356.9 _{3/2}	5s5p5d 384255 $^o_{5/2}$	1.06E+11	1.07E+11	0.42
415.599	$5s5p^2$ 153628.1 _{5/2}	$4f5p^2 \ 394242^o_{5/2}$	8.00E+09	9.44E+09	-0.63
421.169	5s5p ² 220463.2 _{1/2}	5s5p5d 4578981/2	2.80E+10	3.16E+10	-0.02
421.247	5s5p ² 184888.4 _{5/2}	5s5p5d 422273 ^o / ₇ / ₂	3.50E+10	5.60E+10	0.15
422.810	5s5p ² 191315.3 _{1/2}	$4f5p^2 427829^{o_{1/2}}$	1.90E+10	7.89E+10	0.29
422.987	$5s^25d$ 264176 5r/s	$5s^25f500588^\circ$	2.36E+11	2.42E+11	0.78
423 800	$5s^2 5n^2 P^0$	$5s^25d 264176 5$	2.202111	$1.07E \pm 11$	0.44
423.090	5° 5P 1 3/2 5° ² 5d 264176 5	5°25£ 4007040	2 20E + 10	6 75E - 00	0.77
	18-30 2041/D. 3r /o	38-31 499 / 84 _{5/2}	2.20E+10	0./JE+09	-0.77
424.432	$5 \cdot 5 \cdot 2 \cdot 2 \cdot 2 \cdot 1 \cdot 1 \cdot 5 \cdot 5 \cdot 2 \cdot 2$	5 - 5 - 5 1 4557000	E 200 . 10		
424.432	$5s5p^2 220463.2_{1/2}$	5s5p5d 455788 _{3/2}	5.60E+10	1.10E+10	-0.56
424.432 424.945 424.945	$\frac{585p^2}{585p^2} \frac{220463.2_{1/2}}{220463.2_{1/2}}$	$5s5p5d 455788^{o}_{3/2} 4f5p^2 426634^{o}_{3/2}$	5.60E+10 1.50E+10	1.10E+10 2.24E+10	-0.36
424.432 424.945 424.945 426.161	$\begin{array}{c} 5850^{2} \ 220463.2_{1/2} \\ 585p^{2} \ 220463.2_{1/2} \\ 585p^{2} \ 191315.3_{1/2} \\ 585p^{2} \ 143356.9_{3/2} \end{array}$	$\begin{array}{l} 5s5p5d \ 455788^{o}_{3/2} \\ 4f5p^2 \ 426634^{o}_{3/2} \\ 4f5p^2 \ 378012^{o}_{5/2} \end{array}$	5.60E+10 1.50E+10 1.20E+10	1.10E+10 2.24E+10 1.13E+10	-0.36 -0.21 -0.54
424.432 424.945 424.945 426.161 431.037	$\begin{array}{c} 5s5p^2 \ 220463.2_{1/2} \\ 5s5p^2 \ 191315.3_{1/2} \\ 5s5p^2 \ 143356.9_{3/2} \\ 5s5p^2 \ 184888.4_{5/2} \end{array}$	$\begin{array}{l} 5s5p5d \ 455788^{o}_{3/2} \\ 4f5p^2 \ 426634^{o}_{3/2} \\ 4f5p^2 \ 378012^{o}_{5/2} \\ 5s5p5d \ 416886^{o}_{3/2} \end{array}$	5.60E+10 1.50E+10 1.20E+10 6.00E+09	1.10E+10 2.24E+10 1.13E+10 4.21E+09	-0.36 -0.21 -0.54 -0.96

	T	-:-:-	4	(1)	1(-(-))
$\lambda_{obs} (\mathbf{A})^{a}$	Trans	SITION	gA Dravia ^b	(S ⁻¹) This west-f	$\log (gf)$
422 (02	Lower level	Upper level	Previous ^o	1 nis Work	I his work
433.602	$5s5p^2$ 153628.1 _{5/2}	$5s5p5d 384255_{5/2}^{\circ}$	2.30E+10	1./8E+10	-0.32
435.102	$585p^{-} 184888.4_{5/2}$	$535p50 414/22_{5/2}^{\circ}$	1.11E+11	8.35E+10	0.35
435.742	$585p^{-}$ 221/36.4 _{3/2}	$5s^{2}6p 451225_{3/2}^{3}$	1.50E+10	3.03E+09	-1.07
437.450	$535p41 2/1182.1_{3/2}$	$5s^{-}51499/84_{5/2}^{\circ}$	8./0E+10	9.61E+10	0.40
442.862	$5s^{2}5p^{2}P_{3/2}^{0}$	5s5p4f 2540/0.0 _{5/2}		2./5E+10	-0.10
444./3/	$5s^2 5p {}^2P_{3/2}^0$	$5s^25d 253117.3_{3/2}$	2.005 10	1.6/E+09	-1.29
448.158	$5s5p^2$ 184888.4 _{5/2}	$5s5p5d 408018_{7/2}^{o}$	3.00E+10	1.72E+10	-0.30
448.461	$5s5p^2$ 143356.9 _{3/2}	$5s5p5d 366348_{5/2}^{o}$	5.00E+09	5.15E+09	-0.83
449.135	$5s^25p\ ^2P_{1/2}^0$	5s5p4f 222651.2 _{3/2}		1.95E+10	-0.24
450.990	$5s^25p\ ^2P_{1/2}^o$	5s5p ² 221/36.4 _{3/2}		6.98E+08	-1.56
451.587	$5s^25p\ ^2P^o_{3/2}$	5s5p4f 249703.5 _{3/2}		9.76E+09	-0.55
451.919	5s5p ² 153628.1 _{5/2}	5s5p5d 374907 _{7/2}	2.50E+10	1.87E+10	-0.26
452.290	$5s5p^2 220463.2_{1/2}$	5s5p5d 441561 ^o _{1/2}	3.10E+10	3.16E+10	-0.02
453.589	$5s^25p\ ^2P_{1/2}^o$	$5s5p^2$ 220463.2 _{1/2}		2.69E+09	-1.09
455.550	$5s^25p\ ^2P^o_{3/2}$	5s5p4f 247782 ^o _{5/2}	1.10E+09	4.67E+09	-0.84
457.602	5s5p ² 174459.3 _{3/2}	4f5p ² 392988 ^o _{3/2}	2.80E+10	2.65E+10	-0.10
457.970	5s5p ² 143356.9 _{3/2}	5s5p5d 361709 _{3/2}	2.00E+09	2.13E+09	-1.19
459.950	5s5p ² 174459.3 _{3/2}	$4f5p^2 391878^o_{5/2}$	2.90E+10	4.72E+09	-0.79
465.562	5s5p ² 221736.4 _{3/2}	4f5p ² 436530 ^o _{5/2}	1.40E+10	6.62E+09	-0.67
470.099	5s5p ² 153628.1 _{5/2}	5s5p5d 36634 $8^o_{5/2}$	8.00E+09	5.15E+09	-0.83
471.012	5s5p ² 174459.3 _{3/2}	5s5p5d 386770 ^o _{3/2}	1.20E+10	5.44E+09	-0.75
483.863	5s5p ² 127670.4 _{1/2}	$5p^3 334342^o_{3/2}$	1.00E+10	1.06E+10	-0.45
495.856	5s5p ² 191315.3 _{1/2}	4f5p ² 392988 ^o _{3/2}	1.60E+10	1.24E+10	-0.33
498.255	5s5p4f 225404.0 _{9/2}	$4f5p^2 426108_{11/2}^{o}$	2.60E+10	2.34E+10	-0.07
510.805	5s5p4f 234301.47/2	$4f5p^2 430074^o_{9/2}$	2.30E+10	1.74E+10	-0.17
511.832	$5s^24f^2F^o_{7/2}$	5s5p4f 297037.6 _{5/2}		1.01E+11	0.59
513.434	5s5p4f 231868.2 _{5/2}	$4f5p^2 426634^o_{3/2}$	2.30E+10	4.62E+09	-0.75
514.440	$5s^25p ^2P_{3/2}^o$	5s5p4f 222651.2 _{3/2}		6.85E+10	0.41
515.377	$5s^24f^2P_{5/2}^o$	5s5p4f 293802.3 _{3/2}		7.00E+10	0.44
516.870	$5s^25p {}^2P_{3/2}^{o}$	5s5p ² 221736.4 _{3/2}		2.90E+08	-2.05
519.629	$5s^25d 249703.5_{3/2}$	$5s5p5d 442148_{5/2}^{o}$	2.30E+10	1.51E+10	-0.22
520.300	$5s^25p ^2P_{3/2}^o$	$5s5p^2 220463.2_{1/2}$		2.26E+10	-0.06
520.629	$5s^25d 249703.5_{3/2}$	5s ² 6p 441779 ⁰ _{1/2}	5.00E+09	2.29E+09	-1.05
521.889	$5s^25d 264176.2_{5/2}$	5s5p5d 455788°	3.10E+10	1.83E+10	-0.16
522.697	$5s^25p\ ^2P_{1/2}^o$	$5s5p^2$ 191315.3 ^{1/2}		3.03E+10	0.07
523.601	$5s5p^2$ 143356.9 _{3/2}	$5p^3 334342^{\circ}_{2/2}$	1.30E+10	2.13E+10	-0.09
523.703	$5s5p^2$ 184888.4 _{5/2}	$5p^3 375835^9_{2/2}$	2.40E+10	1.81E+10	-0.15
527.468	$5s5p^2$ 127670.41/2	$5p^3 317255^{9}_{51/2}$	1.20E+10	1.06E+10	-0.45
528.240	5s5p4f 260578 _{9/2}	5s5p5d 449886 ^o	6.10E+10	3.88E+09	-0.75
531.949	5s5p4f 216947.8=/2	$4f5p^2 404935^{\circ}_{2}$	2.60E+10	2.30E+10	-0.01
534.050	$585p^2 174459.3_{2/2}$	5s5p5d 361709°	3.00E+09	1.58E+09	-1.18
536 731	$5s5p^2$ 174459 $3_{3/2}$	$5n^3 360769^o$	2 10F+10	1.30E+09 1 40F+10	-0.24
537.262	5s5p4f 234301 4 _{7/2}	$4f5n^2 420432^o$	2.10E+10	2.42E+10	0.01
538 134	5s5p4f 279688 7-10	$415p^{-4}20452_{5/2}$ $4f5n^{2}465514^{o}$	5.20E+10	2.42E+10 2.75E+10	0.09
541 283	5s5p4f 279000.77/2	$415p^{-}405514_{7/2}$ $4f5p^{2}436530^{o}$	3.20E+10 3.00E+10	2.75E+10	0.14
541 605	$5s^2 4f^2 F^0$	5s5n4f 284406.6	5.006+10	$6.26E \pm 10$	0.17
5/1 976	55 = 15/2 5s5n/f 210005 4	Af5n ² A025220	210E + 10	1 520110	-0.19
J44.0/0 545 227	5°54f 5°50	$+13p +03323_{5/2}^{-}$	2.10E+10	1.J2E+10 1.12E+11	-0.18
J4J.227	$58 + \Gamma_{7/2}$	155p ² 427225 ⁰	4 20E + 10	1.13E+11 2.20E+10	0.70
540.190	585p41 244249 _{9/2}	$413p^{-} 42/333_{9/2}^{\circ}$	4.20E+10	3.30E+10	0.10
J40.333	525p2 152628 1	$413p^{-} 427277_{7/2}$	5.50E+10	2.91E+10 2.64E+00	0.10
547.010	5 246 250	$5p^{\circ} 550027_{5/2}^{\circ}$	7.00E+09	2.04E+09	-0.94
547.212	$5s^{-41} F_{7/2}^{o}$	5\$5p41 284406.6 _{7/2}	1.200 10	9.50E+09	-0.37
547.450	5s5p4t 224528.1 _{7/2}	$415p^{\circ} 40^{\prime} 192_{9/2}^{o}$	1.30E+10	1.09E+10	-0.32

Table A.5: Continued.

λ_{obs} (Å) ^a	Transition		$qA(s^{-1})$		$\log(qf)$
000 ()	Lower level	Upper level	Previous ^b	This work ^c	This work ^c
548.998	5s5p4f 219995.47/2	4f5p ² 402146 ^o _{9/2}	3.20E+10	3.23E+10	0.16
550.021	5s5p4f 245526.87/2	4f5p ² 427335 ^o _{9/2}	1.90E+10	1.79E+10	-0.11
550.214	5s5p4f 245526.87/2	$4f5p^2 427277^{o}_{7/2}$	2.30E+10	1.39E+10	-0.21
550.528	5s5p4f 245526.87/2	$4f5p^2 427173^{o}_{5/2}$	2.60E+10	1.87E+10	-0.08
552.400	5s5p4f 219995.47/2	$4f5p^2 401024_{5/2}^{o}$	1.40E+10	8.27E+09	-0.42
553.360	5s5p ² 153628.1 _{5/2}	$5p^3 334342^o_{3/2}$	1.60E+10	1.91E+10	-0.09
553.794	5s5p4f 246760.0 _{11/2}	$4f5p^2 427335^o_{9/2}$	4.30E+10	3.34E+10	0.18
554.192	5s5p4f 285070.3 _{9/2}	$4f5p^2 465514_{7/2}^{o}$	8.30E+10	4.49E+10	0.33
555.810	$5s^24f^2F^o_{5/2}$	5s5p4f 279688.77/2		1.01E+10	-0.33
557.119	5s5p4f 247782 _{5/2}	$4f5p^2 427277^o_{7/2}$	2.00E+10	4.85E+09	-0.66
557.579	5s5p4f 246760 _{11/2}	$4f5p^2 426108_{11/2}^{o}$	5.60E+10	4.37E+10	0.30
559.208	5s5p4f 284406.67/2	$4f5p^2 463230^o_{5/2}$	3.00E+10	1.77E+08	-2.10
560.309	$5s^24f^2F^o_{5/2}$	5s5p4f 278244.0 _{5/2}		6.26E+10	0.47
561.708	$5s^25p\ ^2F_{7/2}^o$	5s5p4f 279688.77/2		7.81E+10	0.56
563.001	5s5p4f 224528.1 _{7/2}	4f5p ² 402146 ^o _{9/2}	2.30E+10	9.17E+09	-0.37
563.613	5s5p4f 225404.0 _{9/2}	$4f5p^2 402830_{7/2}^{o}$	2.20E+10	1.17E+10	-0.26
563.847	5s5p4f 219995.47/2	$4f5p^2 397350_{9/2}^{o}$	2.30E+10	3.23E+10	0.16
564.224	5s5p4f 225404.0 _{9/2}	$4f5p^2 402638_{11/2}^{o}$	4.80E+10	3.44E+10	0.20
565.288	5s5p4f 231868.2 _{5/2}	$4f5p^2 408769^o_{7/2}$	3.20E+10	2.06E+10	-0.02
565.483	5s5p4f 224184.0 _{5/2}	$4f5p^2 401024_{5/2}^{o}$	9.00E+09	5.32E+09	-0.59
565.820	5s5p4f 219995.47/2	$4f5p^2 396724_{7/2}^{o}$	1.60E+10	9.74E+09	-0.33
568.073	5s5p4f 216947.8 _{5/2}	$4f5p^2 392986_{7/2}^{o}$	1.20E+10	7.03E+09	-0.47
571.660	5s5p4f 216947.8 _{5/2}	$4f5p^2 391878_{5/2}^{o}$	1.10E+10	8.89E+09	-0.37
573.200	$5s^25p\ ^2P^o_{1/2}$	5s5p ² 174459.3 _{3/2}		9.93E+09	-0.30
574.516	5s5p4f 253117.3 _{3/2}	$4f5p^2 427173^o_{5/2}$	1.60E+10	1.35E+10	-0.20
574.688	5s ² 5d 264176.5 _{5/2}	$5s5p5d 438182_{7/2}^{o}$	1.00E+10	3.31E+10	0.20
575.044	5s5p ² 143356.9 _{3/2}	$5p^3 317255^o_{3/2}$	1.00E+10	2.13E+10	-0.09
575.529	5s5p4f 252879 _{1/2}	$4f5p^2 426634^o_{3/2}$	8.00E+09	8.74E+09	-0.38
577.353	5s5p4f 254070.0 _{5/2}	$4f5p^2 427277^{o}_{7/2}$	1.00E+10	5.26E+09	-0.59
578.399	5s5p4f 234301.47/2	$4f5p^2 407192_{9/2}^{o}$	1.10E+10	4.74E+09	-0.63
579.571	5s5p4f 224184.0 _{5/2}	$4f5p^2 396724^o_{7/2}$	2.10E+10	1.19E+10	-0.23
580.196	5s ² 5d 264176.5 _{5/2}	$4f5p^2 436530^o_{5/2}$	1.20E+10	4.81E+09	-0.62
581.571	5s5p4f 225404.0 _{9/2}	$4f5p^2 397350^o_{9/2}$	9.00E+09	6.85E+09	-0.49
582.786	5s5p4f 222651.2 _{3/2}	$4f5p^2 394242_{5/2}^{o'}$	1.00E+10	4.87E+09	-0.62
586.182	5s5p4f 271182.1 _{3/2}	$5s^26p \ 441779^{o'}_{1/2}$	3.00E+09	8.92E+08	-1.37
589.979	5s5p4f 260578 _{9/2}	$4f5p^2 430074^{o'}_{9/2}$	5.20E+10	4.19E+10	0.33
590.128	5s5p ² 191315.3 _{1/2}	$5p^3 360769^o_{1/2}$	2.00E+09	5.56E+08	-1.53
590.920	5s5p4f 222651.2 _{3/2}	$4f5p^2 391878^o_{5/2}$	5.00E+09	5.15E+09	-0.58
593.610	5s5p4f 224528.17/2	$4f5p^2 392986_{7/2}^{o}$	6.00E+09	5.09E+09	-0.57
603.487	5s5p4f 224528.17/2	$5s5p5d 390232_{9/2}^{o}$	4.00E+09	1.27E+09	-1.15
604.784	5s5p4f 271182.1 _{3/2}	$4f5p^2 436529^{o}_{5/2}$	2.20E+10	9.79E+09	-0.28
611.150	5s5p ² 153628.1 _{5/2}	$5p^3 317255^o_{3/2}$	2.40E+10	1.91E+10	-0.09
613.313	$5s^25p\ ^2P^o_{3/2}$	5s5p ² 191315.3 _{1/2}		8.57E+08	-1.35
613.704	5s5p4f 2517787/2	5s5p5d 414722 ^o _{5/2}	5.00E+09	2.38E+09	-0.89
614.188	5s5p4f 254070.0 _{5/2}	$5s5p5d 416886_{3/2}^{o'}$	6.00E+09	2.88E+09	-0.81
615.100	5s5p4f 245526.87/2	$5s5p5d 408104_{5/2}^{o'}$	1.10E+10	1.09E+10	-0.21
622.460	$5s5p4f\ 224184.0_{5/2}$	$4f5p^2 \ 384837^o_{7/2}$	8.00E+09	1.19E+10	-0.23

$\lambda_{aba} (\text{\AA})^a$	Transition		$aA(s^{-1})$		$\log(af)$
1008 (11)	Lower level	Upper level	Previous ^b	This work ^c	This work ^{c}
622.806	5s5p4f 247782 _{5/2}	5s5p5d 408346 ^o _{2/2}	7.00E+09	1.72E+08	-1.98
623.797	5s5p4f 224528.1 _{7/2}	$4f5p^2 384837^o_{7/2}$	1.20E+10	1.14E+08	-2.24
627.224	5s5p4f 225404.0 _{9/2}	$4f5p^2 384837^o_{7/2}$	4.00E+10	1.19E+08	-2.22
632.843	5s5p4f 219995.4 _{7/2}	$4f5p^2 378012^o_{5/2}$	1.20E+10	7.46E+09	-0.36
638.478	$5s^25p\ ^2P_{2/2}^o$	$5s5p^2$ 184888.4 _{5/2}		6.27E+09	-0.40
641.531	5s5p4f 246760 _{11/2}	$4f5p^2 402638^o_{11/2}$	4.40E+10	3.15E+10	0.27
643.560	5s5p4f 246760 _{11/2}	$4f5p^2 402146_{0/2}^{o}$	3.70E+10	2.75E+10	0.22
648.938	5s5p ² 221736.4 _{3/2}	$5p^3 375835^o_{3/2}$	1.30E+10	5.49E+09	-0.44
653.167	5s5p4f 244249 _{9/2}	$4f5p^2 397350^o_{9/2}$	2.30E+10	7.46E+09	-0.36
655.850	5s5p4f 244249 _{9/2}	$4f5p^2 396724_{7/2}^{o}$	1.40E+10	7.32E+09	-0.34
657.646	5s5p4f 252879 _{1/2}	$4f5p^2 404935_{3/2}^{o}$	9.00E+09	5.27E+09	-0.48
657.864	$5s^24f {}^2F^o_{5/2}$	5s5p4f 251778 _{7/2}	1.00E+09	3.86E+08	-1.57
659.030	$5s5p^2$ 184888.4 _{5/2}	5p ³ 336627 ^o _{5/2}	1.60E+10	1.04E+09	-1.10
662.033	5s5p4f 251778 _{7/2}	$4f5p^2 402830_{7/2}^o$	8.00E+09	3.61E+08	-1.61
664.290	5s5p4f 234301.4 _{7/2}	$4f5p^2 384837_{7/2}^{o}$	2.00E+10	1.95E+09	-0.96
666.144	$5s^24f^2F_{7/2}^o$	5s5p4f 251778 _{7/2}	2.00E+09	7.01E+08	-1.29
674.798	5s5p4f 260578 _{9/2}	$4f5p^2 408769^{o}_{7/2}$	1.10E+10	7.44E+09	-0.31
675.626	$5s^24f^2F_{5/2}^o$	5s5p4f 247782 _{5/2}	7.00E+09	2.82E+08	-1.68
678.145	5s5p4f 245526.8 _{7/2}	$4f5p^2 392986_{7/2}^{o}$	1.20E+10	6.98E+09	-0.33
682.068	5s5p4f 260578 _{9/2}	$4f5p^2 407192_{0/2}^{o}$	1.50E+10	1.14E+10	-0.12
684.024	$5s^25p\ ^2P_{2/2}^o$	$5s5p^2$ 174459.3 _{3/2}		1.06E+08	-2.13
690.791	5s5p4f 216947.8 _{5/2}	$5s5p5d 361709^{\circ}_{2/2}$	3.00E+09	2.98E+09	-0.66
695.090	$5s^24f^2F_{7/2}^o$	5s5p4f 245526.8 _{7/2}		7.39E+08	-1.23
696.996	5s5p4f 246760 _{11/2}	5s5p5d 390232 _{9/2}	2.00E+09	5.07E+09	-0.42
700.298	$5s5p^2$ 174459.3 _{3/2}	5p ³ 317255 ^o _{3/2}	4.00E+09	1.11E+09	-1.21
709.024	$5s5p4f 285070.3_{9/2}$	$4f5p^2 426108^{o}_{11/2}$	1.90E+10	1.19E+10	-0.02
711.208	5s5p4f 234301.4 _{7/2}	5s5p5d 374907 ^o _{7/2}	3.00E+09	2.13E+09	-0.78
712.734	$5s5p^2$ 220463.2 _{1/2}	$5p^3 360769^o_{1/2}$	6.00E+09	2.99E+09	-0.64
743.330	$5s^24f^2F_{5/2}^o$	5s5p4f 234301.4 _{7/2}		1.64E+08	-1.83
753.911	$5s^24f^2F_{7/2}^{o}$	5s5p4f 234301.4 _{7/2}		8.95E+08	-1.08
757.023	$5s^24f^2F_{5/2}^{o}$	5s5p4f 231868.2 _{5/2}		1.96E+08	-1.74
768.001	$5s^24f^2F_{7/2}^{o}$	5s5p4f 231868.2 _{5/2}		4.98E+08	-1.32
783.265	$5s^25p {}^2P_{1/2}^{o}$	$5s5p^2$ 127670.4 _{1/2}		2.95E+08	-1.55
794.035	$5s5p^2$ 191315.3 _{1/2}	$5p^3 317255^o_{3/2}$	3.00E+09	8.19E+08	-1.20
797.689	$5s^25p\ ^2P_{2/2}^o$	$5s5p^2$ 153628.1 _{5/2}		9.16E+08	-1.04
801.563	$5s^24f^2F_{5/2}^{o}$	5s5p4f 224528.1 _{7/2}		7.78E+08	-1.09
803.775	$5s^24f^2F_{5/2}^{o}$	5s5p4f 224184.0 _{5/2}		5.18E+08	-1.26
808.124	$5s^24f^2F_{7/2}^{o}$	5s5p4f 225404.0 _{9/2}		8.49E+08	-1.04
813.880	$5s^24f^2F_{7/2}^{0}$	5s5p4f 224528.1 _{7/2}		4.59E+08	-1.30
831.779	$5s^24f^2F_{5/2}^{o}$	5s5p4f 219995.47/2		1.80E+08	-1.70
853.412	$5s^24f^2F_{5/2}^{o}$	5s5p4f 216947.8 _{5/2}		9.14E+07	-1.97
868.878	$5s^25p P_{2/2}^{0/2}$	5s5p ² 143356.9 _{3/2}		8.37E+07	-2.00
870.394	$5s5p^2 221736.4_{3/2}$	$5p^3 336627^o_{5/2}$	4.00E+09	2.35E+09	-0.52
1006.004	$5s^25p\ ^2P^o_{3/2}$	$5s5p^2$ 127670.4 _{1/2}		2.70E+07	-2.37

Table A.5: Continued.

- ^a Gayasov et al. (1998) and Churilov and Joshi (2001)
- ^b Churilov and Joshi (2001)
- ^c Transition probabilities (gA) and oscillator strengths $(\log(gf))$ calculated using HFR method (this work)

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$\lambda_{obs} (\mathbf{A})^a$	Tran	sition	gA	(S^{-1})	$\log(gf)$
160.066	Lower level	Upper level	Previous ^a	This work ^o	This work ^o
160.066	$5s^{2} {}^{1}S_{0}$	$5s6p P_1^{-1}$	3.47E+10	3.27E+10	-0.90
162.335	$5s^{2} S_{0}^{1}$	$5s6p {}^{3}P_{1}^{o}$	1.17E+10	9.95E+09	-1.40
236.951	$5s5p {}^{3}P_{0}^{o}$	5s6s ${}^{3}S_{1}$	2.08E+10	2.44E+10	-0.68
240.719	$5s5p {}^{3}P_{1}^{o}$	$5s6s {}^{3}S_{1}$	5.57E+10	6.66E+10	-0.24
255.507	$5s5p {}^{3}P_{2}^{o}$	5s6s ${}^{3}S_{1}$	8.28E+10	9.84E+10	-0.02
272.757	$5s5p \ ^{1}P_{1}^{o}$	5s6s ${}^{1}S_{0}$	4.00E+10	4.35E+10	-0.30
280.140	$5s5p \ ^{1}P_{1}^{o}$	5s6s 3S_1	2.40E+09	1.90E+09	-1.63
335.339	$5p^2 {}^3P_1$	4f5d ${}^{3}D_{2}^{o}$	1.30E+10	1.02E+10	-0.75
335.638	5s5p ³ P ₁ ^o	5s5d ¹ D ₂	9.80E+09	3.13E+09	-1.29
337.243	$5p^2 {}^1D_2$	4f5d ³ D ₃ ^o	3.48E+10	2.70E+10	-0.33
363.174	$5p^2 {}^1D_2$	5p5d ${}^{1}F_{3}^{o}$	5.74E+10	5.76E+10	0.06
366.409	5s5p ³ P ₀	$5s5d {}^{3}D_{1}$	5.09E+10	3.95E+10	-0.11
369.473	$5p^{2^{-3}}P_{2}$	5s6p ³ P ₁ ^o	6.50E+09	4.31E+09	-1.09
374.335	$5s5p {}^{3}P_{1}^{o}$	$5s5d^{3}D_{2}$	1.17E+11	9.19E+10	0.28
374.675	$5p^{2} P_{1}$	$5p5d {}^{3}P_{1}^{o}$	6.89E+10	5.30E+10	0.06
375.498	$5s5p {}^{3}P_{1}^{o}$	$5s5d^{3}D_{1}^{1}$	3.33E+10	3.31E+09	-1.29
376.079	$4f5p {}^{3}G_{4}$	$4f5d {}^{1}H^{2}$	3.88E+10	3.50E+10	-0.12
380.193	$5n^2 {}^3P_0$	$5n5d {}^{3}D_{1}^{9}$	1.23E+11	9.12E+10	0.31
383 615	$5p^{2} {}^{1}D_{2}$	$5n5d {}^{3}D_{2}^{o}$	1 92E+11	1 57E+11	0.54
383 615	$4f5n {}^{3}F_{2}$	$4f5d {}^{3}D_{2}^{9}$	3.62E+10	3.84E+10	-0.05
384 314	$4f5n {}^{3}F_{2}$	$4f5d {}^{3}D^{9}$	8.63E+10	7.01E+10	0.05
386 512	$4f5n {}^{3}G$	$4f5d {}^{3}D^{9}$	3.56E+10	3.24E+10	-0.13
388 989	5s5n ³ P ^o	$415a D_3$ 4f5n 3D_1	$1.11E \pm 10$	3.24E+10 3.95E+10	-0.11
300.202	$535P I_0$ $5n^2 3P$	$5n5d {}^{3}D^{0}$	1.11E+10 1.10E+11	3.75±10	0.28
303 523	$5p^{2} I_{1}$ $5p^{2} I_{D}$	5p5d D_2 5p5d $^3D^o$	1.10L+11 4.86E+10	$2.80E \pm 10$	0.28
303.608	$\frac{3p}{4f5n}$ $\frac{3G}{3G}$	Эрэц D ₂ 4f5d ³ н⁰	4.00L+10 8 11E+10	2.00E+10 6.67E+10	-0.10
304 300	$415p G_3$	$4150 II_4$	2.71E+10	0.07E+10 2 38E+10	0.20
305 086	415p 03	$5_{s}5f^{3}E^{0}$	2.712 ± 10 1.64E±11	$2.38E \pm 10$ 1 23E ± 11	-0.24
395.980	$5350 D_1$	$5_{0}5_{1}^{3}E^{0}$	1.04L+11	1.23E + 11	0.40
390.378	$3530 D_2$	3831 Γ ₃ 4f54 ³ Εθ	2.03E+11	1.99E + 11	0.07
390.803	415p O_3	4130 Γ_2	2.94E+10	2.36E+10	-0.24
398.083	$413p^{-3}G_4$	$4130^{-1}G_{4}$	4.01E+10	4.33E+09	-0.90
398.805	$415p {}^{\circ}G_4$	$4150^{\circ}H_5^{\circ}$	2.11E+11	5.21E+10	0.11
399.220	$415p^{\circ}G_{3}$	$4150 {}^{3}G_{4}^{3}$	1.51E+11	1.16E+11	0.45
399.250	$3s3p P_1^{\circ}$	$415p {}^{\circ}D_1$	7.20E+09	7.82E+09	-0.73
399.397	$3s3d ^{\circ}D_3$	5851 $^{\circ}F_4^{\circ}$	4.08E+11	3.20E+11	0.88
399.622	$415p {}^{9}F_{3}$	4f5d ${}^{3}H_{4}^{3}$	6.5/E+10	4.44E+10	0.04
400.254	$415p^{-3}F_{3}$	$4f5d {}^{9}F_{3}^{9}$	9.40E+10	2.3/E+10	-0.23
401.941	4f5p ${}^{3}F_{2}$	4f5d ${}^{3}F_{2}^{0}$	9.51E+10	7.66E+10	0.28
402.758	$4f5p {}^{3}G_{4}$	$4f5d^{-3}H_{4}^{0}$	7.46E+10	5.21E+10	0.11
404.193	$5p^2 {}^{\circ}P_2$	$5p5d {}^{1}F_{3}^{o}$	1.52E+11	1.23E+11	0.48
404.193	$5s5p {}^{3}P_{1}^{o}$	$4f5p {}^{3}D_{2}$	1.20E+10	1.11E+10	-0.57
405.283	$4f5p {}^{3}F_{3}$	$4f5d {}^{1}G_{4}^{o}$	2.42E+10	1.92E+10	-0.31
407.301	$5s5p {}^{3}P_{2}^{o}$	$5s5d {}^{3}D_{3}$	1.20E+10	1.48E+11	0.55
408.517	$4f5p {}^{3}G_{4}$	$4f5d {}^{1}G_{4}^{o}$	3.18E+10	2.23E+10	-0.24
411.346	$5s5p \ {}^{3}P_{2}^{o}$	5s5d $^{3}D_{2}$	3.04E+10	2.41E+10	-0.23
417.550	$5s5p \ ^{1}P_{1}^{o}$	$5s5d \ ^1D_2$	1.53E+11	6.57E+10	0.24
420.342	$5p^2 \ ^3P_2$	$5p5d {}^{3}P_{2}^{o}$	1.18E+11	8.33E+10	0.35
421.312	4f5p ¹ F ₃	4f5d ³ D ₃ ^o	2.98E+10	2.66E+10	-0.12
422.185	4f5p ¹ F ₃	4f5d ${}^{3}D_{2}^{o}$	1.61E+10	3.19E+09	-1.04
422.704	$5p^2 \ ^3P_1$	5p5d $^{1}D_{2}^{o}$	7.97E+10	4.91E+10	0.13
422.969	4f5p ³ D ₃	4f5d ${}^{3}P_{2}^{o}$	6.93E+10	5.67E+10	0.19

Table A.6: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in La X.

λ_{aba} (Å) ^a	Trans	Transition		(s^{-1})	$\log(af)$
, (008 (1 1)	Lower level	Upper level	Previous ^a	This work ^{b}	This work ^{b}
424.142	$585d {}^{1}D_{2}$	$\frac{585f^{1}F_{3}^{0}}{585f^{1}F_{3}^{0}}$	3.10E+11	1.26E+11	0.54
426.173	$4f5p^{3}F_{4}$	$4f5d^{3}D_{2}^{o}$	2.73E+10	2.44E+10	-0.17
426.610	$5p^{2} {}^{1}D_{2}$	$5p5d {}^{1}D_{2}^{o}$	4.30E+10	3.85E+10	0.03
429.695	$5n^2 {}^{3}P_2$	$5n5d^{3}D_{2}^{o}$	7.31E+10	6.11E+10	0.23
432.371	$4f5n^{3}D_{2}$	$4f5d^{3}D_{3}^{2}$	2.98E+10	2.66E+10	-0.12
432.647	$4f5n {}^{1}F_{2}$	$4f5d^{3}P_{4}^{0}$	6.23E+10	1.82E+10	-0.27
433 343	$4f5n {}^{1}G_{4}$	$4f5d {}^{1}H^{9}$	2.41E+11	1.82E+10	0.73
434 237	$4f5n {}^{3}F_{4}$	$4f5d {}^{3}G^{o}$	1 79E+11	1 31E+11	0.58
435 104	$4f5n {}^{1}F_{2}$	$4f5d {}^{3}G^{0}$	6.72E+10	3.35E+10	-0.02
435 386	$5n^{2} {}^{1}D_{2}$	$5n5d {}^{3}F_{2}^{o}$	3 32E+10	1 74E+10	-0.29
437 515	$5\mathbf{p}^2 \mathbf{D}_2$ $5\mathbf{p}^2 \mathbf{I} \mathbf{S}_2$	$4f5d {}^{1}P_{2}^{0}$	5.32E+10	7 20E+07	-2 72
437 765	$4f5n {}^{3}F_{4}$	$415d \ ^{3}F^{0}$	6.33E+10	1.82E+10	-0.27
440 709	$415p T_4$ 4f5n ¹ Fa	$415d^{-1}4$	$4.74E \pm 10$	$4.84E \pm 10$	0.15
441 273	415p + 13 $4f5n + 3F_4$	$415d \ ^{3}H^{o}$	4.74E+10 6.04E+10	5.79E+10	0.13
441 561	$415p \ 1_4$ $4f5n \ ^3G_2$	$415d \ ^{3}H^{o}$	$3.12E \pm 11$	2.79E+10 2.49E+11	0.23
441 845	$415p G_5$	$415d \ {}^{3}G^{o}$	7.22+11	$6.11E \pm 10$	0.26
444 310	$415p O_5$ $4f5n {}^3D_2$	$4150 \ O_5$	6.69E±10	$1.18E \pm 10$	-0.44
445 263	$5s5n {}^{3}P^{0}$	$4150 P_4$	$1.00E \pm 10$	1.16E+10 1.26E+10	-0.44
445.205	$4f5n {}^{1}F_{2}$	$415p D_3$ $4f5d ^1G^0$	1.00E+10	6.32E±00	-0.72
447.004	415p - 13 $4f5p - 3G_{-}$	$4150 O_4$	2.402+09	0.32E+09 2 08E+10	-0.12
449.110	$415p \ O_5$	$415d \ 11_5$	2.90E+10	2.00E+10	-0.19
457 348	$5s5n {}^{3}P^{0}$	$4150 G_4$	1 30E±09	0.24E109	-0.71
458 894	$5s5p T_1$ 5s5d ³ D ₂	415p + 12 $4f5d + ^3P^0$	1.50E+09 1.51E+10	9.00 ± 00 1 44E+10	-0.33
460 645	$5350 D_2$ $5n^2 D_2$	5n5 d ${}^{3}\text{F}^{o}$	1.31E+10	1.44E+10 1.06E+10	-0.35
462 509	$\frac{5p}{4f5s}$ $\frac{1}{5}$	$5p5d T_2$ 5s5d 1D_2	$3.69E \pm 10$	$2.04E \pm 10$	-0.40
462.806	$4158 \ 1_3$	$3530 D_2$	3.09E+10 3.08E+10	2.04E+10 2.21E+07	3 15
402.800	$5 \text{ s5d }^{3}\text{D}_{4}$	$5s6n {}^{3}P^{0}$	$3.98E \pm 10$ 1 01E ± 10	2.212 ± 07 1 $44E\pm10$	-0.32
463.871	$4f5n {}^{1}G$	250р 1 ₁ Лf5d ³ H ⁰	1.912 ± 10 $1.48E\pm10$	1.44E+10 1.43E+10	-0.32
405.871	$5 \text{ s5d }^{3}\text{D}_{2}$	$4150 11_5$ $4150 30^{\circ}$	$1.43E \pm 10$ 1.84E \pm 10	1.43L+10 1 0/E+10	-0.33
465 442	$5850 D_3$	$5c6n {}^{3}D^{0}$	1.04L+10 3.04E+10	1.94E+10 2 54E+10	-0.20
405.442	$5850 D_2$ 585n ³ P ^o	$500 P_{1}$ $5n^{2} {}^{3}P_{2}$	3.04E+10 1 21E+10	2.34L+10 1.07E+10	-0.07
475.104	$4f5p {}^{1}G$	$\frac{3p}{4}$ $\frac{1}{6}$	1.21E+10 3.83E+10	1.07E+10 3.60E+10	-0.45
470.980	415p O_4	$4150 O_4$	3.83E+10 1 58E+10	3.00L+10 2 40E+10	0.10
409.300 510 164	$413p D_2$ $5a5p ^1 P^0$	$4130 \Gamma_3$	$1.36E \pm 10$	2.49L+10	-0.13
511 229	$353p r_1$	413p D_2	1.83E+10	1.20L+10 5.74E+00	-0.29
511.520	4138 Γ_3 $4f5_{0}^{3}E^{0}$	$5_{0}5_{0}4_{3}$	3.30E+09	3.74E+09	-0.04
515.001	4138 Γ_4	$5_{2}5_{4}^{3}D$	4.03E+10	4.20E+10	0.24
515.852	4158 ${}^{\circ}F_{2}^{\circ}$	$5s5d$ $^{\circ}D_2$	0.40E+09	0.03E+09	-0.37
J1/./43 510.060	4138 [~] Γ ³ 4 f5 _c ³ Ε ⁰	5,543D	3.19E+10	3.30E+1U	0.14
J10.000 510 740	4138 F ₂	$\mathbf{J}\mathbf{S}\mathbf{J}\mathbf{U}^{*}\mathbf{D}_{1}$	2.00E+10	2.77E+10	0.03
J18.742	$5530 {}^{2}D_{2}$	$3 \sup^{-1} \mathbf{P}_{1}^{\circ}$	2.33E+10	1.03E+10	-0.37
519.525	$55^{-1}S_0$	$3s_{2}p^{-1}P_{1}^{2}$	4.08E+10	3.88日+10 1.62日 - 10	0.19
520.204	$413p^{3}G_{4}$	$5p30$ $^{\circ}F_{3}^{\circ}$	1./0E+10	1.03E+10	-0.13
532.394	$3SOP P_0^{\circ}$	$Sp^{-} P_1$	1.//E+10	1.38E+10	-0.25
555.922	$SSD P_2^{o}$	Sp P_2	4.15E+10	5.42E+10	0.15

Table A.6: Continued.

$\lambda = (\mathring{A})^a$	Trans	sition	a A	$aA(s^{-1})$	
\mathcal{N}_{ODS} (11)	I ower level	Unner level	Previous ^a	This work ^b	This work ^b
539 881	$\frac{4 \text{f} 5 \text{n}^{3} \text{G}}{4 \text{f} 5 \text{n}^{3} \text{G}}$	$\frac{5 \text{ ppcl level}}{5 \text{ p5d }^3 \text{ F}^o}$	$2.48E\pm10$	$2.52E\pm10$	
540 570	$415p^{-3}G_{2}$	$5p5d F_4$ $5p5d ^3F^o$	1 38F±10	$1.39E \pm 10$	-0.19
545 280	$5s5n {}^{3}P^{0}$	$5p3d T_2$ $5p^2 T_2$	1.30E+10 1.44E+10	9.56E±09	-0.38
548 507	$335p I_1$	$\frac{3p}{4f5n} \frac{1}{G}$	1.44L110 8.00E±00	7.78E±00	-0.30
551 812	$4138 \Gamma_3$ 5.5n ³ D ⁰	$5n^2 {}^3\mathbf{P}$	$1.12E \pm 10$	7.782+09	-0.44
552 212	$355p T_1$	$5p I_1$ $4f5n I_C$	$1.12E \pm 10$ 6 70E ± 00	5.892 ± 09	-0.41
554 079	4138 Γ_4	413p O_4	0.70E+09	3.60E+09	-0.30
564.078	4138 F_{3}	$413p^{-}D_{2}$	4.20E+09	1.90E+09	-1.04
564.514	$3S3p^{-}P_{1}^{*}$	$3p^{-3}S_{0}$	1.30E+10	1.1/E+10	-0.25
564.420	4158 ° F_2^3	$415p \circ D_1$	7.60E+09	2.51E+07	-2.93
565.211	$5850 ^{\circ}\text{D}_2$	$spsd {}^{\circ}D_{3}^{\circ}$	1.59E+10	8.89E+09	-0.37
570.315	4f5s ${}^{3}F_{2}^{2}$	$4f5p^{-3}D_3$	9.00E+08	6.59E+08	-1.48
572.636	4f5s ${}^{3}F_{3}^{0}$	4f5p ${}^{3}D_{3}$	1.28E+10	9.16E+09	-0.34
572.788	4f5s ${}^{1}F_{3}^{0}$	$4f5p^{-1}G_4$	4.27E+10	3.33E+10	0.23
573.066	$5s5d {}^{3}D_{3}$	$5p5d {}^{9}D_{3}^{o}$	2.30E+10	1.72E+10	-0.07
574.298	4f5s ${}^{3}F_{2}^{o}$	$4f5p {}^{3}D_{2}$	1.57E+10	1.23E+10	-0.20
574.803	4f5s ${}^{3}F_{4}^{o}$	$4f5p {}^{3}G_{5}$	7.12E+10	5.75E+10	0.47
576.663	4f5s ${}^{3}F_{3}^{o}$	$4f5p {}^{3}D_{2}$	2.80E+09	2.03E+09	-0.99
576.813	4f5s ${}^{3}F_{4}^{o}$	$4f5p {}^{3}D_{3}$	8.70E+09	6.38E+09	-0.49
578.908	$4f5s {}^{1}F_{3}^{o}$	$4f5p {}^{1}D_{2}$	9.30E+09	7.90E+09	-0.39
583.864	4f5s ${}^{3}F_{3}^{o}$	4f5p ³ F ₄	3.82E+10	3.15E+10	0.22
588.205	4f5s ${}^{3}F_{4}^{o}$	4f5p ³ F ₄	1.67E+10	1.40E+10	-0.13
590.741	$4f5s \ {}^{3}F_{2}^{o}$	4f5p ¹ F ₃	2.20E+10	1.84E+10	-0.01
593.244	$4f5s {}^{3}F_{3}^{o}$	4f5p ¹ F ₃	7.30E+09	6.77E+09	-0.43
599.168	$4f5s {}^{1}F_{3}^{o}$	4f5p ³ D ₃	9.50E+09	7.97E+09	-0.36
606.422	5s5d ³ D ₃	$5p5d \ {}^{3}F_{4}^{o}$	3.39E+10	2.08E+10	0.09
621.777	4f5s ${}^{1}F_{3}^{o}$	4f5p ¹ F ₃	1.13E+10	7.97E+09	-0.36
621.949	5s5d ¹ D ₂	5p5d ${}^{1}F_{3}^{o}$	1.78E+10	7.11E+09	-0.37
626.590	5s5p ³ P ₁ ^o	$5p^2 {}^{3}P_0$	1.06E+10	8.70E+09	-0.32
627.593	$5s5p^{3}P_{2}^{o}$	$5p^{2} {}^{1}D_{2}$	1.41E+10	9.98E+09	-0.25
636.241	$5s5p^{3}P_{2}^{o}$	$5p^2 {}^3P_1$	1.28E+10	1.05E+10	-0.22
654.123	$5s5p {}^{1}P_{1}^{\bar{o}}$	$5p^2 {}^3P_2$	8.10E+09	5.18E+09	-0.45
679.395	$4f5s^{3}F_{3}^{o}$	$4f5p \ {}^{3}G_{4}$	6.30E+09	4.67E+09	-0.49
685.284	4f5s ${}^{3}F_{4}^{o}$	$4f5p {}^{3}G_{4}$	2.17E+10	1.88E+10	0.13
687.918	4f5s ${}^{3}F_{2}^{\bar{o}}$	$4f5p {}^{3}F_{2}$	8.10E+09	7.78E+09	-0.25
688.537	4f5s ${}^{3}F_{3}^{o}$	$4f5p^{-3}F_{-3}$	5.90E+09	5.12E+09	-0.44
691.309	$4f5s {}^{3}F_{2}^{o}$	$4f5p^{-3}F_{2}$	7.50E+09	6.25E+09	-0.34
694.584	$4f5s {}^{3}F_{4}^{0}$	$4f5p^{-3}F_{-3}$	1.29E+10	1.02E+10	-0.13
703.283	$4f5s {}^{3}F_{2}^{0}$	$4f5n^{3}G_{2}$	1.13E+10	9.14E+09	-0.17
706.822	$4f5s {}^{3}F_{2}^{0}$	$4f5n^{3}G_{2}$	7.30E+09	6.80E+09	-0.29
717.070	$4f5s {}^{1}F_{2}^{o}$	$4f5n^{3}G_{4}$	6.10E+09	5.26E+09	-0.39
727 272	$4f5s {}^{1}F^{o}$	$4f5n {}^{3}F_{2}$	5.20E+09	5 58E+09	-0.35
746 148	$5s^2 {}^1S_2$	$5s5n {}^{3}P^{0}$	9.00F+08	5.30E+08	-1 32
747 702	$4f5s$ $^{1}F^{o}$	$4f5n {}^{3}G_{2}$	5 70F+00	4 69F+09	-0.40
800.455	$5s5n {}^{1}P^{o}$	$5n^2 {}^1D_2$	5.30E+09	4.31E+09	-0.35
000.100		~r ~2			0.00

Table A.6: Continued.

^a Ryabtsev et al. (2002)

λ_{obs} (Å) ^a		$\log(qf)$	
	HFR	MCDHF	AMBiT
La V			
398.531	-1.40	-1.50	-1.16
421.547	-1.55	-1.57	-1.42
423.074	-0.13	-2.10	0.50
432.108	0.76	0.57	0.84
435.275	1.02	1.04	0.96
436.135	0.87	0.80	0.72
436.843	0.51	0.55	0.63
450.405	-0.27	0.33	-0.24
463.848	-0.50	0.49	0.36
476.667	-1.71	-0.33	-1.26
482.164	-0.94	-0.65	-0.79
482.434	-0.72	-0.79	-1.78
498.081	-1.22	-0.90	-1.20
499.028	-0.48	-0.22	-0.19
503.583	-1.32	-1.01	-1.25
508.147	-3.30	-4.82	-3.16
525.712	-1.70	-1.37	-1.37
526.755	-1.18	-0.94	-1.10
531.069	-0.89	-0.70	-0.87
533.233	-0.89	-0.57	-0.71
540.203	-1.19	-1.23	-1.00
544.805	-1.79	-0.89	-1.48
547.437	-1.47	-1.07	-1.18
570.903	-2.35	-2.00	-2.07
593.181	-1.88	-1.64	-1.88
597.698	-2.75	-2.52	-2.68
600.009	-2.11	-1.84	-2.04
600.237	-2.26	-2.11	-2.12
611.695	-2.66	-2.63	-2.38
617.600	-3.29	-2.11	-3.35
620.981	-2.79	-3.00	-3.12
686.469	-4.70	-4.68	-4.83
699.449	-1.44	-1.09	-1.22
824.156	-1.52	-1.27	-1.40

Table A.7: Comparison between oscillator strengths (log(gf)) obtained in the present work using HFR, MCDHF and AMBiT methods for a sample of lines in La V, La VIII and La X.

Table A.7: Continued.

$\lambda_{obs} (\text{\AA})^a$	$\log(qf)$			
	HFR	MCDHF	AMBiT	
La VIII				
370.024	-2.10	-1.19	-0.52	
379.061	-0.41	-0.22	0.07	
391.082	-1.11	-0.47	0.05	
395.969	-0.20	-0.33	-0.13	
398.509	0.04	-0.24	-0.62	
400.709	-0.44	-0.61	0.16	
401.128	-0.41	-0.50	-0.55	
401.29	-0.07	0.28	0.09	
401.373	-0.02	-0.08	0.02	
407.895	0.62	0.41	0.75	
408.095	-0.73	-0.71	-0.02	
408.959	-1.08	-1.30	-0.51	
411.267	-2.82	-2.64	-0.10	
418.762	0.05	0.55	0.72	
435.017	-0.42	-0.19	-0.02	
438.465	0.17	0.39	0.42	
443.03	-0.56	-0.71	-0.70	
445.851	-0.41	-0.42	-0.55	
446.161	-0.14	0.07	0.41	
451.14	-0.33	0.02	-0.04	
454.23	-0.19	-0.47	-0.16	
455.551	-1.38	-1.29	-0.36	
455.956	-1.83	-1.66	-2.05	
458.423	-0.04	0.25	0.26	
459.727	-0.49	-0.56	-0.39	
466.767	-1.00	-1.00	-0.20	
477.454	-1.18	-0.89	-0.87	
479.129	-0.37	-0.07	-1.11	
489.046	-2.70	-1.96	-2.91	
492.517	-0.86	-0.39	-0.54	
503.887	-0.60	-0.87	-0.30	
504.545	-0.18	-0.22	-0.10	
507.156	-1.79	-1.59	-1.56	
508.511	-0.92	-0.47	-0.60	
511.63	-1.12	-0.91	-1.01	

λ_{obs} (Å) ^a	$\log(qf)$			
	HFR	MCDHF	AMBiT	
514.659	-0.02	0.13	0.10	
521.397	0.24	0.24	0.34	
528.453	-2.38	-2.88	-2.31	
544.375	-2.38	-1.98	-2.74	
559.753	-2.07	-2.89	-1.69	
561.708	-1.04	-0.62	-0.73	
567.753	-0.51	-0.26	-0.41	
573.071	-0.73	-0.48	-0.66	
575.852	-0.96	-0.82	-0.80	
584.76	-0.21	-0.04	-0.11	
589.188	-1.88	-3.09	-1.46	
599.598	-1.47	-1.12	-1.98	
603.291	-0.26	-0.14	-0.20	
603.881	-0.64	-0.45	-0.52	
664.918	-0.66	-0.53	-0.56	
669.155	-0.53	-0.41	-0.42	
680.391	-1.36	-1.25	-1.24	
684.932	-1.57	-1.09	-1.89	
699.114	-2.43	-2.18	-2.32	
714.96	-1.60	-1.30	-1.58	
797.561	-0.76	-0.64	-0.69	
800.581	-1.78	-1.66	-1.70	
842.378	-1.78	-1.66	-1.49	
847.275	-2.10	-1.92	-2.26	
870.654	-1.88	-1.80	-1.71	
890.432	-1.67	-1.45	-1.56	
1052.091	-2.62	-2.81	-2.46	
1145.559	-2.55	-2.49	-2.36	
La X				
335.339	-0.75	-0.99	-0.67	
337.243	-0.33	-0.19	-0.25	
363.174	0.06	0.34	0.12	
366.409	-0.11	-0.40	-0.11	
374.335	0.28	0.18	0.31	
374.675	0.06	-0.46	0.14	
375.498	-1.29	-0.57	-0.26	

Table A.7: Continued.

$\lambda_{obs} (\text{\AA})^a$		$\log(qf)$	
000 ()	HFR	MCDHF	AMBiT
380.193	0.31	0.30	0.38
383.615	0.54	0.34	0.62
384.314	0.20	0.46	0.22
388.989	-0.11	-0.29	-0.34
390.180	0.28	-0.07	0.37
393.523	-0.18	0.27	-0.09
394.309	-0.24	-0.30	-0.28
396.865	-0.24	-0.28	-0.21
398.083	-0.96	-0.80	-0.61
398.865	0.11	0.69	0.65
399.220	0.45	0.16	0.50
399.250	-0.73	-0.45	-0.48
400.254	-0.23	-0.27	0.35
401.941	0.28	0.02	0.35
402.758	0.11	0.24	0.21
404.193	0.48	-0.03	0.57
405.283	-0.31	0.28	-0.21
407.301	0.55	0.70	0.63
408.517	-0.24	0.24	-0.07
411.346	-0.23	-0.34	-0.17
417.550	0.24	0.58	0.65
420.342	0.35	0.03	0.45
422.185	-1.04	-1.13	-0.35
422.704	0.13	-0.04	0.23
422.969	0.19	0.18	0.15
426.173	-0.17	-0.12	-0.19
426.610	0.03	0.27	0.14
429.695	0.23	0.01	0.32
432.371	-0.12	-0.34	-0.18
432.647	-0.27	0.19	0.17
433.343	0.73	0.86	0.79
434.237	0.58	0.82	0.68
435.386	-0.29	-0.19	-0.19
437.765	-0.27	0.41	0.11
440.709	0.15	0.18	0.14
441.273	0.23	-0.28	0.23

Table A.7: Continued.

λ_{obs} (Å) ^a		$\log(qf)$	
	HFR	MCDHF	AMBiT
441.561	0.87	1.00	0.95
441.845	0.26	0.18	0.35
444.310	-0.44	0.40	-0.10
447.604	-0.72	-0.43	-0.69
449.110	-0.19	-0.03	-0.05
453.110	-0.71	-0.79	-0.75
457.348	-1.53	-1.22	-1.44
458.894	-0.33	-0.17	-0.07
460.645	-0.46	-0.34	-0.36
462.509	-0.19	-0.01	0.15
463.871	-0.33	-0.78	-0.28
473.164	-0.45	-0.63	-0.29
476.986	0.10	0.24	0.16
510.164	-0.29	-0.84	-0.16
511.328	-0.64	-0.89	-0.52
514.661	0.24	0.15	0.29
515.852	-0.57	-0.74	-0.44
517.743	0.14	-0.37	0.22
518.068	0.05	0.06	0.14
519.525	0.19	0.20	0.31
521.162	-0.15	-0.64	-0.17
532.394	-0.25	-0.28	-0.12
533.922	0.15	0.03	0.29
539.881	0.07	0.43	0.05
540.570	-0.19	-0.19	-0.21
545.280	-0.38	-0.28	-0.26
548.507	-0.44	-0.52	-0.35
551.812	-0.41	-0.46	-0.28
552.313	-0.56	-0.63	-0.49
554.078	-1.04	-0.08	-1.01
564.314	-0.25	-0.29	-0.13
564.420	-2.93	-1.90	-0.72
570.315	-1.48	-1.40	-1.24
572.636	-0.34	-0.23	-0.18
572.788	0.23	0.21	0.35
573.066	-0.07	-0.53	0.01

Table A.7: Continued.

$\lambda_{obs} ({ m \AA})^a$	$\log(gf)$				
	HFR	MCDHF	AMBiT		
574.298	-0.20	-0.33	-0.11		
574.803	0.47	0.43	0.58		
576.663	-0.99	-0.08	-1.12		
576.813	-0.49	-0.21	-0.46		
578.908	-0.39	-0.60	-0.27		
583.864	0.22	0.17	0.32		
588.205	-0.13	-0.18	0.01		
590.741	-0.01	-0.06	0.10		
593.244	-0.43	-0.57	-0.39		
599.168	-0.36	-0.45	-0.32		
621.777	-0.36	-0.29	-0.11		
621.949	-0.37	-0.77	-0.03		
626.590	-0.32	-0.37	-0.19		
627.593	-0.25	-0.17	-0.15		
636.241	-0.22	-0.29	-0.11		
654.123	-0.45	-0.17	-0.37		
679.395	-0.49	-0.48	-0.34		
685.284	0.13	0.05	0.24		
687.918	-0.25	-0.36	-0.14		
688.537	-0.44	-0.49	-0.27		
691.309	-0.34	-0.49	-0.25		
694.584	-0.13	-0.15	-0.03		
703.283	-0.17	-0.23	-0.06		
706.822	-0.29	-0.43	-0.23		
717.070	-0.39	-0.47	-0.32		
727.272	-0.35	-0.51	-0.29		
746.148	-1.32	-1.04	-1.26		
747.702	-0.40	-0.45	-0.24		
800.455	-0.35	-0.34	-0.24		

Table A.7: Continued.

 $^{\rm a}\,$ Extracted from Tables A.1, A.4 and A.6 for La V, La VIII, and La X, respectively.

Appendix B

Comparison of the radiative parameters for Ce V–X ions

Table B.1:	Transition	probabilities ((gA) and	l oscillator	strengths	(log(gf)) for	experimentally	observed
lines in Ce	<i>V</i> .							

) ())((-1)	
$\lambda_{obs} (\mathbf{A})^a$	Trans	sition	gA	(s^{-1})	$\log(gf)$
	Lower level	Upper level	Previous ^a	This work ^o	Previous ^a This work ^b
365.661	$5s^25p^{6-1}S_0$	$5s^25p^36s {}^{3}P_1^0$	2.13E+10	2.74E+10	-0.32
399.361	$5s^25p^{6-1}S_0$	$5s^25p^35d P_1^0$	2.81E+11	2.88E+11	0.76
404.209	$5s^25p^{0-1}S_0$	$5s^25p^36s P_1^{0}$	1.51E+10	2.94E+10	-0.21
482.963	$5s^25p^{6-1}S_0$	$5s^25p^5d^3D_1^o$	9.15E+09	6.68E+09	-0.70
507.683	$4f5s^25p^5 {}^{3}D_1$	$4f5s5p^{6} {}^{3}F_{2}^{o}$	3.44E+10	9.44E+06	-3.25
509.870	$4f5s^25p^5 \ ^3D_2$	$4f5s5p^{6} {}^{3}F_{3}^{o}$	2.97E+10	1.22E+07	-3.13
513.193	$4f5s^25p^5 \ ^3G_5$	$4f5s5p^{6} {}^{3}F_{4}^{o}$	1.31E+11	6.93E+08	-1.36
515.701	$4f5s^25p^5 \ ^3D_2$	$4f5s5p^{6} \ {}^{3}F_{2}^{o}$	1.99E+10	2.75E+07	-2.77
518.645	$4f5s^25p^5 \ ^3G_4$	4f5s5p ^{6 3} F ₃ ^o	9.42E+10	4.10E+08	-1.58
522.234	4f5s ² 5p ⁵ ³ D ₃	4f5s5p ^{6 3} F ₃ ^o	2.32E+10	6.90E+07	-2.35
522.841	$4f5s^25p^5 \ {}^3F_4$	$4f5s5p^{6} {}^{1}F_{3}^{o}$	4.90E+10	7.37E+07	-2.32
529.817	$4f5s^25p^{5-1}D_2$	$4f5s5p^{6} {}^{1}F_{3}^{o}$	3.31E+10	2.79E+08	-1.73
535.649	$4f5s^25p^5 \ ^3F_4$	4f5s5p ⁶ ³ F ₄ ^o	4.12E+10	2.07E+08	-1.84
536.827	4f5s ² 5p ⁵ ³ G ₃	4f5s5p ⁶ ³ F ₂ ^o	4.02E+10	3.28E+08	-1.64
552.134	$5s^25p^{6-1}S_0$	$5s^25p^55d \ {}^{3}P_1^{o}$	5.64E+07	5.88E+07	-2.64
905.114	$5s^25p^55d {}^3P_2^o$	5s ² 5p ⁵ 6p ³ P ₂	1.81E+08	1.13E+09	-0.89
917.980	$5s^25p^55d {}^3P_0^o$	5s ² 5p ⁵ 6p ³ S ₁	1.15E+09	1.51E+09	-0.74
926.103	$5s^25p^55d {}^3P_1^o$	5s ² 5p ⁵ 6p ³ D ₂	2.10E+08	1.68E+08	-1.68
929.993	$5s^25p^55d^3P_2^{o}$	$5s^25p^56p^1P_1$	1.81E+08	3.21E+08	-1.41
936.241	$5s^25p^54f {}^1D_2$	$5s^25p^55d {}^1P_1^o$	4.26E+08	2.23E+08	-1.58
937.539	$5s^25p^55d^3P_3^2$	$5s^25p^56p^3D_3$	2.21E+08	5.27E+08	-1.18
941.960	$5s^25p^55d^3P_1^2$	$5s^25p^56p^3S_1$	2.33E+09	3.22E+09	-0.38
944.710	$5s^25p^55d^3F_4^0$	$5s^25p^56p^3D_3$	2.67E+09	7.40E+09	-0.03
953.946	$5s^25p^55d^3F_3^2$	$5s^25p^56p^3D_3$	3.53E+08	8.88E+08	-0.94
957.514	$5s^25p^55d^3D_0^3$	$5s^25p^56p^3P_1$	4.34E+09	3.81E+09	-0.30
974,399	$5s^25p^55d^3P_0^2$	$5s^25n^56n^3D_2$	8.21E+07	1.80E+07	-2.60
975.215	$5s^25p^55d^3F_2^{o}$	$5s^25n^56n$ ¹ P ₁	3.26E+09	3.78E+09	-0.29
976 416	$5s^2 5p^5 5d^3 F_2^o$	$5s^2 5n^5 6n^3 D_1$	2.49E+09	4 35E+09	-0.25
980.577	$5s^25p^55d^{-1}F_{0}^{0}$	$5s^2 5n^5 6n^3 D_2$	5.33E+09	7.27E+04	-5.00
991 965	$5s^25n^55d^3P_0^2$	$5s^2 5n^5 6n^3 S_1$	1 95E+09	2.60E+09	-0.43
992 129	$5s^25p^55d^3F_2^o$	$5s^{2}5p^{5}6p^{-3}D_{0}$	2.09E+09	2.00E+09	-0.51
1010 827	$5s^25p^55d^3D^9$	$5s^{2}5p^{5}6p^{-3}P_{2}$	8.07E+08	3 33E+09	-0.32
1024 151	$5s^25p^55d^3F_{2}^{o}$	$5s^2 5p^5 6p^3 D_2$	5.08E+08	4 17E+08	-1 19
1043 576	$5s^25p^55d^3F_2^0$	$5s^{2}5p^{5}6p^{-3}S_{1}$	9.37E±07	5.53E+07	-2.06
1051 112	$5s^{2}5p^{5}5d^{3}D^{9}$	$5s^{2}5p^{5}6p^{-3}P_{0}$	9.77E+08	7.67E+08	-0.90
1051.112	$5s^25p^55d^3D^0$	$5s^{2}5p^{5}6p^{-3}D_{0}$	2.07E+08	5.26E+08	-1.08
1114 848	$5s^2 5p^5 6n^3 D_3$	$5s^2 5p^5 6d^3 F_2^{\circ}$	2.07E+06	4.63E+06	-3.05
1141 874	$4f5s^25n^5 {}^3D_2$	$5s^{2}5p^{5}5d^{3}D^{0}$	9.67E+06	1.35E+07	-2.57
1150 225	$5s^25n^55d^3D^o$	$5s^{2}5p^{5}6n^{1}P_{1}$	6.19E+08	6.26E±08	-0.93
1186 865	$4f5s^25n^5 {}^3G_1$	$5s^{2}5p^{5}5d^{3}D^{0}$	2.62E+07	4.83E±07	-1.98
1205 859	$4f5s^25n^5 {}^3D_2$	$5s^{2}5p^{5}5d^{3}D^{0}$	$1.15E \pm 08$	1.03E+07 1.27E+08	-1 54
1203.037	$4153 5p^{-1}D_3$	$5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 5^{\circ} 4^{\circ} D_{3}^{\circ}$	2/8E±08	2.26E±08	-1.34
1234 403	$4153 5p^{-} D_2$ $4f5s^25n^5 {}^3D_2$	$5s^{2}5p^{5}5d^{3}F^{0}$	1.93E±07	2.20E+00 2.21E+07	-2.28
1250 718	$4f5s^25n^5 {}^3G_2$	$5s^25n^55d^3D^0$	5.48F±06	8 14F±05	-2.20
1250.710	$4f5s^25n^5 {}^{3}D$	$5s^{2}5n^{5}5d^{3}D^{0}$	0.6/E+00	1 08F±07	-3.70
1204.429	$4158 \ 5p \ D_1$ $4f58^25p^5 \ ^3E_2$	$5s^{2}5p^{5}5d^{1}F^{0}$	5.16E±07	$3.31E\pm07$	-2.57
1200.303	$4138 \ 5p \ \Gamma_3$ $4f5c^25p^5 \ ^3F$	$5s^{2}5p^{5}5d^{1}F^{0}$	5.02E+08	7.25E+08	-2.10
1299.297	4158 5p Γ_4	$5^{\circ}_{\circ}^{\circ$	3.92E+08	7.23E+06	-0.72
1215 254	4158 5p D_3 4f5 $c^25 n^5 3 D$	$5s 3p 3u r_2$ $5s^2 5r^5 5d 3p_0$	1.10E+07	1.03E+00	-2.08
1215 926	4158 $5p^{-1}D_2$ 4f5 a^25p^5 3E	$5s^{2}5p^{5}5d^{3}D^{0}$	1.4JE+08	1.41E+0.08	-1.41
1313.820	+1.55 5μ F4 Af5e ² 5n ⁵ 3Ε	$5_{8}^{2}5_{7}^{5}5_{4}^{3}D_{3}^{0}$	J.JUE+U0	3 00E + 05	-0.77
1371.330	-1.55 Jp $-1.73Af5e^{2}5e^{5} 3C$	$5_{0}^{2} 5_{0}^{5} 5_{1}^{3} 5_{0}^{2}$	+.0JE+00	5.90E+05	-4.00
1341.040	$4155 \text{ s}^{2}5\text{ s}^{5} ^{3}\text{D}$	5°52222222222	0.56E+07	0.02E+07	-0.//
1350.192	4138 $3p^{-1}D_1$ 4f5 $s^{2}5r^{5}3C$	$5s^{2}5r^{5}54^{3}Ee$	9.30E+U/	9.92E+U/ 4.02E+00	-1.54
1330.338	$4138^{-}3p^{-}$ $3C$	$5s 3p^{2}5d F_{2}^{2}$	J.J4E+U8	4.76E+07	-U.84 1 95
1260 706	$4138^{-}3p^{-}$ G_4	$5s 3p^{2}5d^{2}F_{4}^{3}$	4.23E+U/	4./0E+U/	-1.85
1300./80	$4138^{-}3p^{-1}D_2$	$3s^{-}3p^{\circ}3d^{\circ}D_{3}^{\circ}$	1.30E+04	3.//E+06	-2.96
1302.123	4135-3p° °G ₅	$5s^{-}5p^{-}5d^{-}F_{4}^{-}$	4.02E+08	0.12E+U8	-0.01
1302.403	$3s^{-}3p^{-}6s^{-}P_{2}^{0}$	$5s^{-}5p^{-}6p^{-}P_1$	1.89E+08	9.18E+U/	-1.00
1302.008	4158-5p° °G ₃	$3s^{-}3p^{\circ}3d^{\circ}F_{2}^{\circ}$	3.13E+08	4.43E+08	-0.88
1303.964	$4138^{-3}59^{-3}D_3$	$3s^2 5p^2 5d^2 F_3^2$	/./4E+U/	3.90E+0/	-1./5
1385.346	410s~0p° °D ₃	SS-Sp°Sd °F4	4.38E+06	1.22E+07	-2.42

Table B.1	: Continued	1
Tuble D.1	. Commute	ı.

$\lambda_{obs} (\mathbf{A})^a$	Tran	sition	gA	(s^{-1})	$\log(gf)$
	Lower level	Upper level	Previous ^a	This work ^b	Previous ^a This work ^b
1401.064	4f5s ² 5p ⁵ ³ D ₃	5s ² 5p ⁵ 5d ³ P ₂ ^o	3.20E+08	3.52E+08	-0.96
1401.241	5s ² 5p ⁵ 5d ¹ P ₁ ^o	5s ² 5p ⁵ 6p ¹ S ₀	5.14E+08	2.05E+08	-1.12
1409.195	$4f5s^25p^5 \ ^3D_1$	$5s^25p^55d {}^3P_0^o$	9.21E+07	9.78E+07	-1.51
1414.959	$4f5s^25p^5 {}^3D_2$	$5s^25p^55d {}^{3}P_1^{o}$	1.84E+08	1.96E+08	-1.21
1415.046	$5s^25p^56p^3D_1$	$5s^25p^56d^{-3}D_1^{-2}$	1.15E+09	1.06E+08	-1.44
1423.824	$4f5s^25n^5 {}^3G_2$	$5s^25n^55d^3F_{\circ}^{\circ}$	6.74E+07	7.09E+07	-1.63
1444.901	$4f5s^25p^5 {}^3G_2$	$5s^25n^55d^3F_{c}^{0}$	6.21E+06	4.93E+06	-2.77
1457 288	$5s^2 5n^5 6n^3 D_1$	$5s^25n^56d^3D_0^0$	3 79E+07	9 92E+06	-2.47
1459 172	$5s^{2}5p^{5}6p^{-3}D_{1}$	$5s^2 5p^5 6d^3 F_2^0$	6 25E±09	2 35E±08	-1.07
1473 624	$5s^{2}5p^{5}6p^{-3}D_{1}$	$5^{\circ}_{\circ}^{\circ$	1.28E±00	0.61E±08	-0.54
1475.024	$5s^{2}5p^{5}6p^{-3}S$	$5^{\circ}{}^{2}5^{\circ}{}^{5}6^{\circ}{}^{3}D^{\circ}$	1.20E+09	3.14E+00	-0.04
1475.078	$5s^{2}5p^{5}6p^{1}P$	$5s^{2}5p^{5}6d^{1}P^{0}$	4.13E+09	1.38E + 0.00	-0.01
1407.490	$38 30^{\circ}00^{\circ} F_1$	$5s^{2}5r^{5}5d^{3}Eq$	2.34E+09	1.30E+09	-0.54
1494.330	$4138^{-}3p^{-1}D_2$	$5s^{2}5p^{2}5d^{2}F_{2}^{2}$	7.33E+07	6.49E+07	-1.04
1507.607	$5s^25p^66p^6D_2$	$5s^{2}5p^{6}6d^{6}F_{3}^{2}$	5.4/E+09	4.20E+09	0.13
1508.812	$415s^{2}5p^{5}$ $^{6}F_{4}$	$5s^2 5p^5 5d^{-6}F_3^{-5}$	6.46E+05	1.23E+07	-2.34
1518.101	$5s^{2}5p^{3}6p^{3}S_{1}$	$5s^25p^36d^3P_1^3$	5.10E+09	2.87E+09	-0.02
1532.497	$4f5s^25p^3 {}^{3}F_4$	$5s^25p^55d^3F_4^6$	9.51E+07	6.87E+07	-1.57
1540.573	$5s^25p^56p^3S_1$	$5s^25p^56d^{-3}P_0^{0}$	2.17E+09	1.12E+09	-0.41
1549.367	$5s^25p^56p^3D_3$	$5s^25p^56d {}^3D_3^o$	7.94E+08	8.42E+08	-0.54
1568.225	$4f5s^25p^{5-1}D_2$	$5s^25p^55d \ {}^3F_3^o$	5.83E+06	8.18E+06	-2.48
1575.641	$4f5s^25p^{5-1}D_2$	$5s^25p^55d \ ^3D_1^o$	5.57E+07	8.83E+07	-1.46
1588.325	5s ² 5p ⁵ 6p ¹ P ₁	$5s^25p^56d {}^1D_2^o$	6.21E+09	3.85E+09	0.16
1599.641	5s ² 5p ⁵ 6p ³ D ₂	5s ² 5p ⁵ 6d ³ F ₃ ^o	9.53E+09	2.01E+09	-0.11
1605.239	5s ² 5p ⁵ 6p ³ D ₃	5s ² 5p ⁵ 6d ³ F ₃ ^o	3.93E+08	8.05E+08	-0.51
1608.160	5s ² 5p ⁵ 6p ³ D ₃	$5s^25p^56d {}^3F_4^o$	4.48E+09	4.66E+09	0.26
1610.488	5s ² 5p ⁵ 6p ¹ S ₀	$5s^25p^56d \ ^3D_1^o$	2.02E+09	7.69E+08	-0.55
1621.270	5s ² 5p ⁵ 6p ³ P ₁	$5s^25p^56d {}^3D_2^o$	8.77E+09	1.72E+09	-0.18
1628.460	$5s^25p^56p^3D_2$	$5s^25p^56d {}^{3}F_{2}^{o}$	1.03E+09	2.58E+08	-1.02
1646.859	$5s^25p^56p^3P_2$	$5s^25p^56d {}^3D_3^{o}$	1.36E+09	2.59E+09	0.03
1694.062	$5s^25p^56p^3P_0$	$5s^25p^56d {}^{1}P_1^{o}$	2.42E+09	1.05E+09	-0.37
1720.590	$5s^25p^56p^3P_2$	$5s^25p^56d^3P_2^{1}$	3.68E+08	1.05E+09	-0.31
1741.233	$4f5s^25p^5 {}^3F_2$	$5s^25p^55d^3D_9^2$	4.32E+06	4.29E+06	-2.68
1765.111	$4f5s^25p^5 {}^{3}F_{4}$	$5s^25n^55d^3D_0^3$	4.77E+06	8.96E+06	-2.35
1767.382	$4f5s^25p^{5-1}D_2$	$5s^25n^55d^3P_1^9$	1.93E+05	5.77E+05	-3.52
1779 403	$5s^2 5n^5 6n^3 P_0$	$5s^25n^56d^{-3}P_{-}^{0}$	645E+07	1 46E+08	-1 14
1824 990	$5s^2 5n^5 6s^1 P^0$	$5s^{2}5n^{5}6n^{3}P_{0}$	7.85E+08	4 57E+08	-0.59
1841 673	$4f5s^25n^5 {}^3G_0$	$5s^{2}5n^{5}5d^{3}F^{9}$	3.65E+05	1.80E+04	-5.00
1955 172	$4f5s^25n^5 {}^3G_2$	$5s^{2}5p^{5}5d^{3}F^{0}$	4 31E+06	7.67E+05	-3 30
1001 325	$5e^25n^56e^{-3}P^0$	$5s^{2}5p^{5}6p^{3}P_{3}$	2.00E±08	7.07E+08	-0.36
2018 054	$5s^{2}5p^{5}6s^{1}p^{0}$	$5s^{2}5p^{5}6p^{3}P$	2.00L+08	1.74E+08	-0.50
2018.034	$5s^{2}5p^{5}6s^{3}P^{0}$	$5s 5p 6p 1_2$ $5c^2 5p^5 6p 1_2$	2.78E+08	4.00E+08	-0.55
2070.643	$5s 3p 0s F_1$ $5s^2 5r^5 6s ^3 D^9$	$5s^{2}5r^{5}6r^{3}D^{0}$	4.07E+00	$2.23E \pm 0.08$	-0.79
2081.231	$35 \text{ Sp} \cdot 05 \text{ P}_0$	$5s^{2}5r^{5}5d^{3}Eq$	1.2/E+09	4.90E+06	-0.52
2093.999	$4138^{-}3p^{*} F_{3}$	$5s^{-}5p^{*}5u^{*}F_{3}^{*}$	4.03E+00	2.92E+00	-2.00
2115.855	$55^{-}5p^{+}05^{-}P_{2}^{-}$	$5s^{-}5p^{*}op^{-}P_{1}$	3.82E+07	5.14E+07	-1.47
2150.091	$4158^{-}5p^{-}F_4$	$5s^{-}5p^{-}5d^{-}F_{3}^{0}$	1./3E+03	1.0/E+U0	-2.89
2135.022	$5s^2 5p^6 6s^6 P_1^6$	$5s^25p^66p^6D_2$	6.5/E+06	1.36E+09	0.00
2141.969	415s ² 5p ³ 9 F ₃	$5s^25p^55d^3F_4^0$	6.00E+08	5.10E+06	-2.39
2143.434	$5s^{2}5p^{3}6s^{3}P_{1}^{0}$	$5s^25p^36p^3P_1$	1.54E+09	4.17E+08	-0.56
2146.057	$5s^25p^36s {}^1P_1^o$	5s ² 5p ³ 6p ¹ P ₁	1.12E+09	9.90E+08	-0.14
2155.318	$5s^25p^56s\ ^3P_2^o$	$5s^{2}5p^{5}6p^{-3}D_{3}$	8.67E+06	1.65E+09	0.06
2178.222	$4f5s^25p^5 \ ^3F_4$	$5s^25p^55d \ {}^3F_4^o$	3.07E+08	3.25E+06	-2.57
2360.591	$5s^25p^56s\ ^3P_2^o$	5s ² 5p ⁵ 6p ³ D ₂	5.02E+08	8.47E+07	-1.11
2398.256	$5s^25p^56s {}^1P_1^o$	5s ² 5p ⁵ 6p ³ D ₂	2.10E+08	3.58E+08	-0.42
2432.642	$5s^25p^56s {}^3P_0^o$	5s ² 5p ⁵ 6p ³ D ₁	1.10E+09	5.63E+08	-0.39
2466.420	5s ² 5p ⁵ 6s ³ P ₂ ^o	5s ² 5p ⁵ 6p ³ S ₁	5.95E+08	7.52E+08	-0.14
2518.038	5s ² 5p ⁵ 6s ³ P ₁ ^o	5s ² 5p ⁵ 6p ³ D ₁	2.13E+10	1.96E+08	-0.81

^{*a*} Wajid et al. (2021)

Table B.2: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in Ce VI.

λ_{aba} (Å) ^a	Т	ransition	$aA(s^{-1})$		$\log(af)$	
, 100s (1 1)	Lower level	Upper level	Previous ^a	This work ^b	Previous ^a	This work ^{b}
311.989	$5s^25p^5 {}^2P_{1/2}^o$	$5s^25p^46s \ 346509_{1/2}$	9.60E+09	1.82E+10		-0.62
321.678	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 6s 310870 _{3/2}	9.90E+09	8.81E+09		-0.91
323.020	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 6s 309578 _{5/2}	5.00E+10	5.48E+10		-0.11
328.952	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 6s 303995 _{1/2}	1.95E+10	2.64E+10		-0.41
332.998	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^46s \ 300301_{3/2}$	2.51E+10	2.71E+10		-0.39
345.313	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 6s 288592 _{1/2}	5.50E+09	8.05E+09		-0.89
351.019	$5s^25p^5 {}^2P_{1/2}^{o}$	5s ² 5p ⁴ 6s 310870 _{3/2}	4.28E+10	4.87E+10		-0.10
359.699	$5s^25p^5 {}^2P_{1/2}^o$	5s ² 5p ⁴ 6s 303995 _{1/2}	2.53E+10	3.23E+10		-0.25
361.140	$5s^25p^5 {}^2P_{3/2}^{o}$	5s ² 5p ⁴ 6s 276899 _{3/2}	6.92E+10	8.63E+10		0.17
364.543	$5s^25p^5 {}^2P_{1/2}^o$	5s ² 5p ⁴ 6s 300301 _{3/2}	1.60E+09	6.69E+09		-0.92
366.323	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 6s 272983 _{5/2}	5.60E+09	6.46E+09		-0.94
370.565	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 269857 _{1/2}	2.60E+09	1.10E+10		-0.71
372.816	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 268229 _{5/2}	4.00E+08	2.70E+11		0.71
383.440	$5s^25p^5 {}^2P_{1/2}^{o}$	5s ² 5p ⁴ 5d 286782 _{3/2}	1.88E+11	2.73E+08		-2.19
385.839	$5s^25p^5 {}^2P_{3/2}^{o'}$	5s ² 5p ⁴ 5d 259175 _{5/2}	6.41E+11	2.56E+09		-1.30
387.312	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 258190 _{3/2}	2.46E+11	1.83E+11		0.54
388.784	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 257211_{1/2}$	2.24E+11	1.82E+11		0.53
390.048	$5s^25p^5 {}^2P_{1/2}^{o}$	5s ² 5p ⁴ 5d 282363 _{3/2}	1.86E+11	3.01E+08		-2.14
398.545	$5s^25p^5 {}^2P_{1/2}^{o'}$	5s ² 5p ⁴ 6s 276899 _{3/2}	4.00E+08	1.10E+08		-2.64
399.448	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 250345 _{3/2}	8.64E+10	2.18E+10		-0.32
410.053	$5s^25p^5 {}^2P_{1/2}^{o}$	$5s^25p^45d \ 269857_{1/2}$	1.57E+11	1.43E+11		0.48
426.917	$5s^25p^5 {}^2P_{3/2}^{o'}$	$5s^25p^45d \ 234237_{5/2}$	6.10E+09	3.89E+09		-1.03
430.653	$5s^25p^5 {}^2P_{1/2}^{o'}$	5s ² 5p ⁴ 5d 258190 _{3/2}	1.37E+10	7.73E+08		-1.76
432.481	$5s^25p^5 {}^2P_{1/2}^{o'}$	$5s^25p^45d \ 257211_{1/2}$	6.70E+09	1.78E+09		-1.40
439.717	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 227419 _{5/2}	7.00E+08	1.99E+09		-1.29
444.942	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 224748_{5/2}$	9.50E+09	2.62E+09		-1.16
445.713	$5s^25p^5 {}^2P_{1/2}^o$	5s ² 5p ⁴ 5d 250345 _{3/2}	2.50E+10	1.32E+10		-0.46
446.633	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 223899 _{3/2}	1.00E+08	2.63E+06		-4.00
463.376	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 215807 _{3/2}	1.40E+09	4.94E+08		-1.85
467.558	$5s^25p^5 \ ^2P^o_{3/2}$	5s ² 5p ⁴ 5d 213877 _{5/2}	4.00E+09	3.04E+09		-1.06
474.178	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 210891_{3/2}$	9.30E+09	5.64E+09		-0.78
475.343	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 210374_{5/2}$	1.09E+10	4.87E+09		-0.84
478.387	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 209037_{1/2}$	1.00E+08	2.00E+09		-1.44
485.117	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 206135_{1/2}$	8.70E+09	2.05E+09		-1.21
487.679	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 205055 _{3/2}	2.20E+09	9.96E+08		-1.51
505.268	$5s^25p^5 {}^2P^o_{1/2}$	5s ² 5p ⁴ 5d 223899 _{3/2}	4.00E+08	1.22E+08		-2.40
526.234	$5s^25p^5 {}^2P^o_{3/2}$	$5s^25p^45d \ 190030_{1/2}$	2.00E+08	3.80E+07		-2.85
526.811	$5s^25p^5 {}^2P^o_{1/2}$	5s ² 5p ⁴ 5d 215807 _{3/2}	2.00E+08	2.51E+08		-2.06
531.723	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 188068 _{3/2}	1.00E+08	5.88E+07		-2.66
533.058	$5s^25p^5 {}^2P^o_{3/2}$	5s ² 5p ⁴ 5d 187597 _{5/2}	2.00E+08	1.43E+08		-2.27
546.288	$5s^25p^5 {}^2P^o_{1/2}$	$5s^25p^45d \ 209037_{1/2}$	1.00E+08	4.04E+07		-2.80
555.100	$5s^25p^5 {}^2P^o_{1/2}$	5s ² 5p ⁴ 5d 206135 _{1/2}	5.00E+08	7.08E+07		-2.57
558.436	$5s^25p^5 {}^2P^o_{1/2}$	5s ² 5p ⁴ 5d 205055 _{3/2}	1.00E+08	5.60E+07		-2.66
623.379	$5s^25p^5 {}^2P^o_{3/2}$	5s5p ⁶ 160416 _{1/2}	2.60E+09	1.04E+09		-1.28
743.876	$5s^25p^{5-2}P_{1/2}^o$	5s5p ⁶ 160416 _{1/2}	1.20E+09	5.50E+08		-1.42

- ^a Churilov and Joshi (2000)
- ^b Transition probabilities (gA) and oscillator strengths $(\log(gf))$ calculated using HFR method (this work)

λ_{obs} (Å) ^a	Trar	nsition	\overline{qA}	$aA(s^{-1})$		$\log(qf)$	
000 ()	Lower level	Upper level	Previous ^b	This work ^c	Previous ^b	This work ^{c}	
262.945	$5s^25p^4 {}^3P_2$	$5s^25p^36s {}^1P_1^o$	3.48E+08	4.14E+08	-2.46	-2.40	
273.144	$5s^25p^4 {}^3P_0$	$5s^25p^36s {}^1P_1^o$	3.63E+08	1.55E+08	-2.40	-2.80	
281.211	$5s^25p^4 {}^3P_1$	$5s^25p^36s {}^1P_1^o$	1.38E+09	2.98E+09	-1.80	-1.49	
282.720	$5s^25p^4 {}^3P_1$	$5s^25p^36s {}^1P_1^o$	6.75E+09	8.20E+09	-1.10	-1.04	
288.039	$5s^25p^4 {}^1D_2$	$5s^25p^36s {}^1P_1^o$	1.72E+10	2.37E+10	-0.68	-0.57	
289.619	$5s^25p^{4} {}^1D_2$	$5s^25p^36s {}^1P_2^o$	8.85E+09	7.70E+09	-0.97	-1.05	
289.655	$5s^25p^4 {}^3P_2$	$5s^25p^36s {}^1P_2^o$	1.09E+10	1.39E+10	-0.87	-0.79	
290.291	$5s^25p^4 {}^3P_0$	$5s^25p^36s {}^1P_1^o$	1.38E+10	3.97E+09	-0.77	-1.28	
292.123	$5s^25p^4$ 3P_2	$5s^25p^36s {}^1P_3^{o}$	3.84E+10	8.00E+10	-0.32	-0.03	
295.643	$5s^25p^4 \ ^3P_2$	$5s^25p^36s \ ^1P_1^o$	8.04E+09	8.10E+09	-0.99	-1.01	
298.564	$5s^25p^4 \ ^3P_2$	$5s^25p^36s \ ^1P_2^{o}$	1.77E+10	3.74E+10	-0.52	-0.34	
299.416	$5s^25p^4 \ ^3P_1$	$5s^25p^36s \ {}^1P_1^{o}$	3.75E+09	3.10E+09	-1.38	-1.42	
299.891	$5s^25p^4 \ ^3P_1$	$5s^25p^36s \ ^1P_0^o$	5.31E+09	6.34E+09	-1.16	-1.11	
307.170	$5s^25p^{4\ 1}D_2$	$5s^25p^36s \ ^1P_1^o$	1.29E+10	2.74E+09	-0.76	-1.45	
308.620	$5s^25p^4 \ ^3P_0$	$5s^25p^36s \ ^1P_1^o$	8.64E+08	4.56E+09	-1.92	-1.17	
311.984	$5s^25p^4 \ ^3P_1$	$5s^25p^36s \ ^1P_2^o$	1.16E+10	1.74E+10	-0.79	-0.64	
314.984	$5s^25p^4 \ ^3P_2$	$5s^25p^36s \ ^1P_1^o$	5.28E+10	9.96E+09	-0.12	-0.87	
318.946	$5s^25p^4 \ ^3P_1$	$5s^25p^36s \ ^1P_1^o$	4.47E+10	3.18E+10	-0.18	-0.35	
319.459	$5s^25p^4 \ ^3P_2$	$5s^25p^36s \ ^1P_2^o$	1.27E+09	6.07E+09	-1.71	-1.04	
320.412	$5s^25p^{4\ 1}D_2$	$5s^25p^36s \ ^1P_2^o$	1.10E+11	1.03E+11	0.22	0.16	
322.340	$5s^25p^4 \ ^3P_1$	$5s^25p^36s \ ^1P_2^o$	3.87E+09	8.36E+09	-1.23	-0.93	
323.433	$5s^25p^{4\ 1}D_2$	$5s^25p^36s \ ^1P_3^o$	8.75E+09	7.39E+09	-0.88	-0.98	
327.760	$5s^25p^{4\ 1}D_2$	$5s^25p^36s \ ^1P_1^o$	6.48E+09	3.30E+09	-0.99	-1.31	
329.744	$5s^25p^4 \ ^3P_0$	$5s^25p^36s \ ^1P_1^o$	2.22E+10	8.73E+09	-0.45	-0.89	
331.353	$5s^25p^{4\ 1}D_2$	$5s^25p^36s \ ^1P_2^o$	7.00E+09	4.00E+09	-0.95	-1.22	
341.580	$5s^25p^4 \ ^3P_1$	$5s^25p^36s \ ^1P_1^o$	9.00E+09	3.54E+09	-0.81	-1.25	
487.862	$5s^25p^4 \ ^3P_2$	$5s^25p^35d \ ^5D_1^o$		3.29E+08		-1.97	
554.709	$5s^25p^4 \ ^3P_1$	$5s^25p^35d\ ^5D_1^o$		4.40E+08		-1.74	
571.236	$5s^25p^4 \ ^3P_2$	$5s5p^{5} {}^{3}P_{1}^{o}$	2.87E+09	2.43E+09	-0.85	-0.97	
572.450	$5s^25p^{4\ 1}D_2$	$5s5p^{5}$ ¹ P_1^o	4.29E+09	3.89E+09	-0.68	-0.76	
581.935	$5s^25p^{4\ 1}D_2$	$5s^25p^35d \ {}^5D_1^o$		1.60E+09		-1.14	
606.582	$5s^25p^4 \ ^3P_1$	$5s5p^{5} {}^{3}P_{0}^{o}$	1.19E+09	1.04E+09	-1.18	-1.29	
611.894	$5s^25p^4 \ ^3P_2$	$5s5p^{5} {}^{3}P_{2}^{o}$	4.20E+09	3.53E+09	-0.63	-0.75	
621.703	$5s^25p^4 \ ^3P_0$	$5s5p^{5} {}^{3}P_{1}^{o}$	1.01E+09	9.46E+08	-1.23	-1.31	
665.114	$5s^25p^4 \ ^3P_1$	$5s5p^{5} {}^{3}P_{1}^{o}$	7.38E+08	6.61E+08	-1.32	-1.41	
704.617	$5s^25p^4 \ ^1D_2$	$5s5p^{5} {}^{3}P_{1}^{o}$	2.55E+08	2.78E+08	-1.72	-1.74	
720.884	$5s^25p^4 \ ^3P_1$	$5s5p^{5} {}^{3}P_{2}^{o}$	1.34E+09	1.26E+09	-0.99	-1.06	
721.828	$5s^25p^{4-1}S_0$	$5s5p^5 {}^1P_1^o$	2.71E+08	3.14E+08	-1.68	-1.68	
737.009	$5s^25p^{4-1}S_0$	$5s^25p^35d\ ^5D_1^o$		2.30E+08		-1.80	
767.520	$5s^25p^4 \ ^1D_2$	$5s5p^{5} {}^{3}P_{2}^{o}$	5.90E+08	5.87E+08	-1.28	-1.34	

^a Tauheed and Joshi (2008)

^b Wajid and Jabeen (2019a)

λ_{obs} (Å) ^a	Trans	ition	gA	(s^{-1})	log	$\overline{(gf)}$
	Lower level	Upper level	Previous ^a	This work ^{b}	Previous ^a	This work ^b
426.529	$5s^25p^3 {}^2D^o_{3/2}$	$5s5p^{4} {}^{2}P_{1/2}$	2.56E+09	2.54E+09	-1.15	-1.39
440.622	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s5p^4 \ ^2S_{1/2}$	1.99E+09	1.66E+09	-1.24	-1.32
486.422	$5s^25p^3 \ {}^4S^{o}_{3/2}$	$5s5p^{4}$ $^{2}D_{5/2}$	9.96E+07	6.56E+07	-2.45	-2.64
489.149	$5s^25p^3 {}^2D_{3/2}^{o}$	$5s5p^{4}$ $^{2}S_{1/2}$	7.78E+09	6.37E+09	-0.55	-0.65
504.486	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s5p^{4} {}^{2}D_{3/2}$	1.35E+09	1.01E+09	-1.29	-1.42
546.290	$5s^25p^3 {}^2D^o_{3/2}$	$5s5p^{4} {}^{2}D_{5/2}$	4.34E+07	3.86E+07	-2.71	-2.77
553.176	$5s^25p^3 {}^2P_{1/2}^{o'}$	$5s5p^{4}$ $^{2}S_{1/2}$	3.70E+09	3.24E+09	-0.76	-0.84
562.502	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s5p^4 \ ^4P_{1/2}$	3.32E+09	2.43E+09	-0.80	-0.96
569.147	$5s^25p^3 {}^2D^o_{5/2}$	$5s5p^4 \ ^2D_{5/2}$	1.04E+10	8.03E+09	-0.29	-0.42
569.147	$5s^25p^3 {}^2D_{3/2}^{o'}$	$5s5p^{4} {}^{2}D_{3/2}$	9.92E+09	7.66E+09	-0.32	-0.44
572.185	$5s^25p^3 \ {}^4S^{o'}_{3/2}$	$5s5p^4 \ ^4P_{3/2}$	6.48E+09	5.00E+09	-0.49	-0.63
622.891	$5s^25p^3 {}^2P^o_{3/2}$	$5s5p^{4}$ $^{2}S_{1/2}$	3.94E+07	1.50E+08	-2.64	-2.08
630.437	$5s^25p^3 \ {}^4S^o_{3/2}$	$5s5p^4 \ ^4P_{5/2}$	4.62E+09	3.54E+09	-0.55	-0.70
644.147	$5s^25p^3 \ ^2D_{3/2}^{o}$	$5s5p^4 \ ^4P_{1/2}$	1.69E+08	1.44E+08	-1.97	-2.08
656.876	$5s^25p^3 {}^2D_{3/2}^{o'}$	$5s5p^4 \ ^4P_{3/2}$	1.52E+06	1.79E+06	-4.00	-3.96
690.223	$5s^25p^3 {}^2D_{5/2}^{o'}$	$5s5p^4 \ ^4P_{3/2}$	2.60E+08	2.67E+08	-1.72	-1.74
718.569	$5s^25p^3 {}^2P^{o'}_{3/2}$	$5s5p^{4}$ $^{2}D_{5/2}$	2.30E+09	2.16E+09	-0.74	-0.80
734.807	$5s^25p^3 {}^2D^o_{3/2}$	$5s5p^4 \ ^4P_{5/2}$	1.33E+09	1.18E+09	-0.96	-1.05
758.682	$5s^25p^3 {}^2P_{3/2}^{o'}$	$5s5p^{4} {}^{2}D_{3/2}$	1.97E+07	3.84E+06	-2.77	-3.51
759.920	$5s^25p^3 {}^2P^o_{1/2}$	$5s5p^4 \ ^4P_{1/2}$	2.38E+08	2.11E+08	-1.68	-1.77
776.746	$5s^25p^3 \ ^2D_{5/2}^{o}$	$5s5p^4 \ ^4P_{5/2}$	5.36E+08	5.22E+08	-1.30	-1.35
777.735	$5s^25p^3 \ ^2P_{1/2}^{o'}$	$5s5p^4 \ ^4P_{3/2}$	6.20E+06	7.11E+06	-3.24	-3.22
923.047	$5s^25p^3 {}^2P_{3/2}^{o'}$	$5s5p^4 \ ^4P_{3/2}$	1.12E+08	9.41E+07	-1.84	-1.97
1084.569	$5s^25p^3 {}^2P^o_{3/2}$	$5s5p^4 \ ^4P_{5/2}$	1.45E+07	1.16E+07	-2.58	-2.74

Table B.4: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in Ce VIII.

^a Wajid and Jabeen (2019b)

Table B.5:	Transition probabilities ((A) and	oscillator	strengths	(log(gf)) for	experimentally	observed
lines in Ce	Х.						

$\lambda_{obs} (\text{\AA})^a$	Tr	ansition	$qA(s^{-1})$		$\log(gf)$	
	Lower level	Upper level	Previous ^a	This work ^{b}	Previous ^a	This work ^b
226.189	$5s^25p\ ^2P^o_{1/2}$	$5s^26s\ ^2S_{1/2}$	4.50E+10	5.43E+10		-0.39
244.683	$5s^25p\ ^2P^{o'}_{3/2}$	$5s^26s\ ^2S_{1/2}$	7.10E+10	8.66E+10		-0.12
335.712	$5s^25p\ ^2P_{1/2}^{o'}$	$5s^25d \ ^2D_{3/2}$	1.16E+11	6.14E+10		0.00
346.792	$5s5p^2 \ ^4P_{3/2}$	$5s5p(^{3}P)5d \ ^{4}D_{5/2}^{o}$	4.20E+10	4.48E+10		-0.11
348.806	$5s5p^2 \ ^4P_{1/2}$	$5s5p(^{3}P)5d \ ^{4}D_{1/2}^{o'}$	9.80E+10	8.47E+10		0.17
350.794	$5s5p^2 \ ^4P_{1/2}$	$5s5p(^{3}P)5d \ ^{4}D_{3/2}^{o'}$	1.16E+11	1.05E+11		0.27
360.090	$5s5p^2 \ ^4P_{3/2}$	$5s5p(^{3}P)5d \ ^{4}D_{7/2}^{o'}$	2.89E+11	1.77E+11		0.53
360.931	$5s5p^2 \ ^4P_{5/2}$	$5s5p(^{3}P)5d \ ^{4}D_{5/2}^{o'}$	8.10E+10	8.74E+10		0.22
372.659	$5s^25p\ ^2P^o_{3/2}$	$5s^25d \ ^2D_{5/2}$	1.93E+11	1.77E+11		0.55
378.142	$5s^25p\ ^2P^{o'}_{3/2}$	$5s^25d \ ^2D_{3/2}$	2.30E+10	2.04E+10		-0.38
388.513	$5s^25p \ ^2P_{1/2}^{o'}$	4f5s(1F)5p 2D _{3/2}	1.00E+10	1.07E+10		-0.64
408.869	$5s^25p\ ^2P_{1/2}^{o'}$	$5s5p^2 \ ^2P_{3/2}$	3.20E+10	2.50E+10		-0.22
409.419	$4f5s^2 {}^2F_{7/2}^{o'}$	$5s^25d \ ^2D_{5/2}$	7.70E+10	7.93E+10		0.30
411.649	$4f5s^2 \ ^2F_{5/2}^{o'}$	$5s^25d \ ^2D_{3/2}$	3.90E+10	2.67E+10		-0.17
413.774	$5s^25p \ ^2P_{1/2}^{o}$	$5s5p^2 \ ^2S_{1/2}$	3.00E+09	3.16E+09		-1.10
443.372	$5s^25p\ ^2P^{o'}_{3/2}$	4f5s(³ F)5p ² D _{5/2}	2.30E+10	2.06E+10		-0.24
446.500	$5s^25p\ ^2P^o_{3/2}$	4f5s(¹ F)5p ² D _{3/2}	7.00E+09	4.90E+09		-0.86
477.297	$5s^25p\ ^2P^o_{3/2}$	$5s5p^2 \ ^2P_{3/2}$	8.30E+10	7.55E+10		0.38
480.196	$5s^25p\ ^2P_{1/2}^{o'}$	$5s5p^2 \ ^2P_{3/2}$	4.20E+10	3.52E+10		0.06
480.196	$5s^25p\ ^2P^o_{3/2}$	$5s5p^2 \ ^2S_{1/2}$	3.00E+09	2.55E+10		-0.08
490.171	$4f5s^2 {}^2F_{5/2}^{o'}$	4f5s(³ F)5p ² D _{5/2}	5.00E+09	2.91E+09		-0.98
493.974	$4f5s^2 {}^2F_{5/2}^o$	4f5s(³ F)5p ² D _{3/2}	4.90E+10	3.52E+10		0.11
495.514	$4f5s^2 {}^2F_{5/2}^{o'}$	4f5s(³ F)5p ² G _{7/2}	1.15E+11	7.51E+10		0.44
496.427	$4f5s^2 {}^2F_{7/2}^{o}$	4f5s(³ F)5p ² D _{5/2}	6.30E+10	4.57E+10		0.22
498.487	$4f5s^2 {}^2F_{7/2}^{o'}$	$4f5s(^{3}F)5p \ ^{2}G_{9/2}$	1.72E+11	1.31E+11		0.69
501.904	$4f5s^2 {}^2F_{7/2}^o$	4f5s(³ F)5p ² G _{7/2}	1.70E+10	1.05E+10		-0.40
507.242	$4f5s^2 {}^2F_{5/2}^{o}$	4f5s(³ F)5p ² F _{7/2}	1.80E+10	1.36E+10		-0.28
513.167	$4f5s^2 {}^2F_{5/2}^{o}$	$4f5s(^{3}F)5p \ ^{2}F_{5/2}$	9.10E+10	7.33E+10		0.46
513.948	$4f5s^2 {}^2F_{7/2}^{o'}$	4f5s(³ F)5p ² F _{7/2}	1.12E+11	8.98E+10		0.55
519.115	$5s^25p\ ^2P_{1/2}^{o}$	$5s5p^2 \ ^2D_{3/2}$	1.40E+10	6.96E+09		-0.54
572.011	$5s^25p\ ^2P^{o}_{3/2}$	$5s5p^2 \ ^2P_{1/2}$	2.00E+09	1.09E+09		-1.30
578.268	$5s^25p\ ^2P^o_{3/2}$	$5s5p^2 \ ^2D_{5/2}$	7.00E+09	3.95E+09		-0.69
717.173	$5s^25p\ ^2P_{1/2}^{o}$	$5s5p^2 \ ^4P_{1/2}$	1.00E+09	4.42E+08		-1.45
732.436	$5s^25p\ ^2P^{o}_{3/2}$	$5s5p^2 \ ^4P_{5/2}$	2.00E+09	1.44E+09		-0.92

^a Joshi et al. (2001)

 $\overline{\lambda_{obs}}$ (Å)^a $\log(qf)$ HFR AMBiT MCDHF Ce V 399.361 0.76 0.75 0.81 482.963 -0.70 -0.43 -0.53 552.134 -2.64 -2.41 -2.52 -1.58 -1.19 936.241 -1.01 1141.824 -2.57 -2.51 -2.48 1186.865 -1.98 -1.85 -1.94 1205.859 -1.54 -1.41 -1.47 1211.818 -1.29 -1.03 -1.15 1234.403 -2.28 -2.18-2.15 1250.718 -3.70 -3.65 -5.58 -2.57 1264.429 -2.42 -2.501286.305 -2.10 -2.12 -2.04 1299.297 -0.72 -0.56 -0.64 -2.55 1309.589 -2.68 -2.30 1315.354 -1.41 -1.30 -1.35 -0.77 1315.826 -0.60 -0.68 1331.550 -4.00 -0.69 -0.76 1341.640 -0.77 -0.71-0.66 -1.54 1356.192 -1.42 -1.47 1358.358 -0.84 -0.75 -0.81 1360.331 -1.85 -1.73 -1.76 1360.786 -2.96 -3.45 -2.95 -0.61 1362.125 -0.51 -0.55 -0.88 -0.85 1362.668 -0.78 1365.964 -1.75 -1.70 -1.73 -2.42 1385.346 -2.87 -2.181401.064 -0.96 -0.82 -0.88 1409.195 -1.51 -1.39 -1.44 1414.959 -1.21 -1.08-1.13 -1.63 -1.52 1423.824 -1.50 -2.77 -2.801444.901 -2.76 -1.64 -1.58 1494.356 -1.52 -2.34 1508.812 -2.52 -2.56 1532.497 -1.50 -1.57 -1.45 1568.225 -2.48 -2.55 -2.43 1575.641 -1.46 -1.51 -1.52 -2.68 1741.233 -2.49 -2.56 -2.35 1765.111 -2.40-2.33 -3.52 1767.382 -3.68 -3.37 -3.92 1841.673 -5.00 -3.16 1955.172 -3.30 -3.13 -3.00 2095.999 -2.66 -2.49 -2.51 -2.39 -2.29 2141.969 -2.49 2178.222 -2.57 -2.45 -2.41

Table B.6: Comparison between oscillator strengths (log gf) obtained in the present work using HFR, MCDHF and AMBiT methods for a sample of lines in Ce V, Ce VIII and Ce X.

Table B.6: Continued.

NobsIngg(y)HFRMCDHFAMBiTCe VIII440.622 -1.32 -2.83 -1.31 486.422 -2.64 -2.31 -2.51 489.149 -0.65 -0.48 -0.65 504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.07 348.806 0.17 0.13 0.19 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 <th>$(\mathring{\Lambda})^a$</th> <th></th> <th>$\log(af)$</th> <th></th>	$(\mathring{\Lambda})^a$		$\log(af)$	
Internal MCDIN AMBIT Ce VIII 440.622 -1.32 -2.83 -1.31 486.422 -2.64 -2.31 -2.51 489.149 -0.65 -0.48 -0.65 504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.66 716.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 92	Λ_{obs} (A)	LIED	MCDUE	AMDIT
Ce VIII 440.622 -1.32 -2.83 -1.31 486.422 -2.64 -2.31 -2.51 489.149 -0.65 -0.48 -0.65 504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X 335.712 0.00 0.01 0.20 346.792 -0.11 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.991 0.22 -0.36 -0.08 <th></th> <th>пгк</th> <th>MCDHF</th> <th>AMDII</th>		пгк	MCDHF	AMDII
440.622 -1.32 -2.83 -1.31 486.422 -2.64 -2.31 -2.51 489.149 -0.65 -0.48 -0.65 504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 $Ce X$ -335.712 0.00 0.01 0.20 346.792 -0.11 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.931 </td <td></td> <td>1.00</td> <td>0.00</td> <td>1.01</td>		1.00	0.00	1.01
486.422 -2.64 -2.31 -2.51 489.149 -0.65 -0.48 -0.65 504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 $Ce X$ 335.712 0.00 0.01 0.20 346.792 -0.11 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.990 0.53 0.67 0.55 360.931 0.22 0.36 -0.32 388.513 <td< td=""><td>440.622</td><td>-1.32</td><td>-2.83</td><td>-1.31</td></td<>	440.622	-1.32	-2.83	-1.31
489.149 -0.65 -0.48 -0.65 504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 $Ce X$ 335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.991 0.22 0.36 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 <t< td=""><td>486.422</td><td>-2.64</td><td>-2.31</td><td>-2.51</td></t<>	486.422	-2.64	-2.31	-2.51
504.486 -1.42 -1.21 -1.23 546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 $Ce X$ 335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.02 378.142 -0.38 -0.56 360.931 0.22 0.36 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419	489.149	-0.65	-0.48	-0.65
546.290 -2.77 -2.51 -2.63 553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -0.11 -0.07 348.806 0.17 355.712 0.00 0.01 0.20 346.792 -0.11 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.931 0.22 0.26 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 <	504.486	-1.42	-1.21	-1.23
553.176 -0.84 -0.67 -0.85 562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -0.11 -0.07 348.806 346.792 -0.11 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.991 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 <	546.290	-2.77	-2.51	-2.63
562.502 -0.96 -0.75 -0.78 569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.9931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10	553.176	-0.84	-0.67	-0.85
569.147 -0.42 -0.22 -0.27 569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.07 -348.806 0.17 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.9931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26	562.502	-0.96	-0.75	-0.78
569.147 -0.44 -0.23 -0.29 572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.991 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.2	569.147	-0.42	-0.22	-0.27
572.185 -0.63 -0.41 -0.47 622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.991 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.37	569.147	-0.44	-0.23	-0.29
622.891 -2.08 -1.83 -2.57 630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.9931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.5	572.185	-0.63	-0.41	-0.47
630.437 -0.70 -0.51 -0.54 644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.9931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.2	622,891	-2.08	-1.83	-2.57
644.147 -2.08 -2.04 -1.94 656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 <	630 437	-0.70	-0.51	-0.54
656.876 -3.96 -2.94 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.66 0.17 493.974 <td>644 147</td> <td>-2.08</td> <td>-2.04</td> <td>-1 94</td>	644 147	-2.08	-2.04	-1 94
0.50.370 -2.390 -2.394 -4.12 690.223 -1.74 -1.49 -1.69 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -355 0.67 0.55 360.90 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 -0.08 -0.12 0.26 493.974 0.11 0.07 0.14 495.514 0.44 <td< td=""><td>656 876</td><td>-2.00</td><td>2.04</td><td>4.12</td></td<>	656 876	-2.00	2.04	4.12
690.223 -1.74 -1.49 -1.09 718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.990 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52	600 222	-3.90	-2.94	-4.12
718.569 -0.80 -0.68 -0.71 734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -0.01 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.990 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69	090.225	-1./4	-1.49	-1.09
734.807 -1.05 -0.93 -0.94 758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -0.01 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 0.06 0.06 0.17 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 </td <td>/18.369</td> <td>-0.80</td> <td>-0.68</td> <td>-0./1</td>	/18.369	-0.80	-0.68	-0./1
758.682 -3.51 -6.18 -2.82 759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -0.01 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.33 <td>/34.80/</td> <td>-1.05</td> <td>-0.93</td> <td>-0.94</td>	/34.80/	-1.05	-0.93	-0.94
759.920 -1.77 -1.57 -1.66 776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X -2.74 -2.79 -2.62 Ce X -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.990 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.33 -0.28 507.242 -0.28 -0.33 -0.25 <td>758.682</td> <td>-3.51</td> <td>-6.18</td> <td>-2.82</td>	758.682	-3.51	-6.18	-2.82
776.746 -1.35 -1.21 -1.27 777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X 335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.990 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.33 -0.28 507.242 -0.28 <	759.920	-1.77	-1.57	-1.66
777.735 -3.22 -3.29 -3.15 923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X 335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 -0.08 -0.12 0.05 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.33 -0.28 507.242 -0.28 </td <td>776.746</td> <td>-1.35</td> <td>-1.21</td> <td>-1.27</td>	776.746	-1.35	-1.21	-1.27
923.047 -1.97 -1.93 -1.82 1084.569 -2.74 -2.79 -2.62 Ce X 335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 -0.08 -0.12 0.05 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46	777.735	-3.22	-3.29	-3.15
1084.569 -2.74 -2.79 -2.62 Ce X335.712 0.00 0.01 0.20 346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 -0.08 -0.12 0.05 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55	923.047	-1.97	-1.93	-1.82
Ce X 335.712 0.000.010.20 346.792 -0.11-0.01-0.07 348.806 0.170.130.19 350.794 0.27-0.110.07 360.090 0.530.670.55 360.931 0.220.220.19 372.659 0.550.41-0.02 378.142 -0.38-0.56-0.32 388.513 -0.64-0.73-0.40 408.869 -0.22-0.36-0.08 409.419 0.300.130.26 411.649 -0.17-0.190.12 413.774 -1.10-1.50-0.84 443.372 -0.24-0.30-0.02 446.500 -0.86-0.93-0.57 477.297 0.380.210.48 480.196 0.060.060.17 480.196 -0.08-0.120.05 490.171 -0.98-2.11-0.67 493.974 0.110.070.14 495.514 0.440.520.64 496.427 0.220.200.26 498.487 0.690.690.80 501.904 -0.40-0.38-0.28 507.242 -0.28-0.33-0.25 513.167 0.460.390.56 513.948 0.550.500.67 519.115 -0.54-0.33-0.18 572.011 -1.30-1.02-1.49	1084.569	-2.74	-2.79	-2.62
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Ce X			
346.792 -0.11 -0.01 -0.07 348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.990 0.53 0.67 0.55 360.990 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 0.06 0.06 0.17 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 $-0.$	335.712	0.00	0.01	0.20
348.806 0.17 0.13 0.19 350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.990 0.53 0.67 0.55 360.991 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 0.06 0.06 0.17 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	346 792	-0.11	-0.01	-0.07
350.794 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.990 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 0.06 0.06 0.17 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	348 806	0.17	0.13	0.19
350.194 0.27 -0.11 0.07 360.090 0.53 0.67 0.55 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 0.08 -0.12 0.05 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	350 704	0.17	0.15	0.17
360.090 0.33 0.07 0.33 360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 -0.08 -0.12 0.05 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	350.794	0.27	-0.11	0.07
360.931 0.22 0.22 0.19 372.659 0.55 0.41 -0.02 378.142 -0.38 -0.56 -0.32 388.513 -0.64 -0.73 -0.40 408.869 -0.22 -0.36 -0.08 409.419 0.30 0.13 0.26 411.649 -0.17 -0.19 0.12 413.774 -1.10 -1.50 -0.84 443.372 -0.24 -0.30 -0.02 446.500 -0.86 -0.93 -0.57 477.297 0.38 0.21 0.48 480.196 0.06 0.06 0.17 480.196 0.08 -0.12 0.05 490.171 -0.98 -2.11 -0.67 493.974 0.11 0.07 0.14 495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	360.090	0.33	0.07	0.55
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	360.931	0.22	0.22	0.19
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	372.659	0.55	0.41	-0.02
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	378.142	-0.38	-0.56	-0.32
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	388.513	-0.64	-0.73	-0.40
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	408.869	-0.22	-0.36	-0.08
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	409.419	0.30	0.13	0.26
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	411.649	-0.17	-0.19	0.12
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	413.774	-1.10	-1.50	-0.84
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	443.372	-0.24	-0.30	-0.02
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	446.500	-0.86	-0.93	-0.57
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	477.297	0.38	0.21	0.48
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	480 196	0.06	0.06	0.17
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	480 196	-0.08	-0.12	0.05
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	400.170	0.00	-0.12	0.05
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	490.171	-0.96	-2.11	-0.07
495.514 0.44 0.52 0.64 496.427 0.22 0.20 0.26 498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	495.974	0.11	0.07	0.14
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	495.514	0.44	0.52	0.64
498.487 0.69 0.69 0.80 501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	496.427	0.22	0.20	0.26
501.904 -0.40 -0.38 -0.28 507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	498.487	0.69	0.69	0.80
507.242 -0.28 -0.33 -0.25 513.167 0.46 0.39 0.56 513.948 0.55 0.50 0.67 519.115 -0.54 -0.33 -0.18 572.011 -1.30 -1.02 -1.49	501.904	-0.40	-0.38	-0.28
513.1670.460.390.56513.9480.550.500.67519.115-0.54-0.33-0.18572.011-1.30-1.02-1.49	507.242	-0.28	-0.33	-0.25
513.9480.550.500.67519.115-0.54-0.33-0.18572.011-1.30-1.02-1.49	513.167	0.46	0.39	0.56
519.115-0.54-0.33-0.18572.011-1.30-1.02-1.49	513.948	0.55	0.50	0.67
572.011 -1.30 -1.02 -1.49	519.115	-0.54	-0.33	-0.18
	572.011	-1.30	-1.02	-1.49
578.268 -0.69 -0.58 -0.46	578.268	-0.69	-0.58	-0.46
717 173 -1 45 -1 27 -1 34	717 173	-1 45	-1 27	-1 34
732.436 -0.92 -0.78 -0.83	732.436	-0.92	-0.78	-0.83

 $^{\rm a}\,$ Extracted from Tables B.1, B.4 and B.5 for Ce V, Ce VIII, and Ce X, respectively.
Appendix C

Comparison of the radiative parameters for Pr V

λ_{obs} (Å) ^a	Transitio	on ^a	$qA(s^{-1})$		log	(qf)	
000 ()	Lower level	Upper level	HFR^{b}	HFR^b	$MCDHF^{b}$	AMBiT ^b	Others
843.783	$5s^25p^64f\ ^2F^o_{5/2}$	5s ² 5p ⁶ 5d ² D _{5/2}	6.78E+07	-2.11	-2.14	-2.00	-1.94^{d}
	~ <i>,</i> _	·					-1.90^{e}
							-2.05^{g}
865.902	$5s^25p^64f\ ^2F^o_{7/2}$	$5s^25p^65d\ ^2D_{5/2}$	1.19E+09	-0.83	-0.86	-0.70	-0.64^{d}
	7						-0.59^{e}
							-0.77^{g}
869.170	$5s^25p^64f\ ^2F^o_{5/2}$	5s ² 5p ⁶ 5d ² D _{3/2}	8.23E+08	-0.99	-1.03	-0.88	-0.81^{d}
							-0.76^{e}
							-0.92^{g}
869.662	$5s^25p^65d\ ^2D_{3/2}$	5s ² 5p ⁶ 6p ² P ^o _{3/2}	1.33E+09	-0.82		-0.90	-0.91^{d}
							-0.91 ^e
							-0.81^{f}
	- 2- 6-12-						-0.84^{g}
896.654	$5s^25p^65d^2D_{5/2}$	$5s^25p^66p\ ^2P^o_{3/2}$	1.10E+10	0.12		0.07	0.06^{a}
							0.06^{e}
							0.16
000 000	5 25 6512D	5 25 66 2D0	5 7 4 E · 00	0.15		0.10	0.09^{g}
922.290	$5s^2 5p^6 5d^2 D_{3/2}$	$5s^2 5p^6 6p^2 P_{1/2}^6$	5./4E+09	-0.15		-0.19	-0.18^{a}
							-0.19 ^e
							-0.08°
1224 070	$5e^{2}5e^{6}6e^{2}D^{0}$	5c25p67c 28	$2.17E \pm 0.0$	0.24		0.40	-0.18°
12/2 775	$5s 5p 6p 1_{1/2}$ $5s^2 5p^6 6p 2 D^0$	$5s^{2}5p^{6}7s^{2}S_{1/2}$	2.17ET09	-0.54		-0.40	-0.31°
1050 000	$5s 5p 0p P_{3/2}$ $5s^2 5p^6 6s^2 S (E-2)$	$5s 3p / s 3_{1/2}$	3.30E+09	-0.07		-0.01	-0.04°
1936.066	$58 \text{ Sp}^{-}08 \text{ S}_{1/2} (F=2)$	$58 \text{Sprop} \mathbf{P}_{3/2}$	2.20E+09	0.17		0.18	0.21°
							0.17^{-1}
							0.13° 0.28 f
							0.28° 0.21 ^g
1958 201	$5s^25n^66s^2S_{1/2}$ (F=3)	$5s^25n^66n^2P^0$	2 28E+09	0.17		0.18	0.21°
1750.201	55 5p 65 51/2 (1-5)	55 5p 6p 1 _{3/2}	2.201107	0.17		0.10	0.21 0.17^d
							0.17 0.15 ^e
							0.28^{f}
							0.21^{g}
2246.759	$5s^25p^66s\ ^2S_{1/2}$ (F=2)	$5s^25p^66p\ ^2P_{1/2}^o$	7.86E+08	-0.19		-0.19	-0.15 ^c
	1 1/2 ()	I I 1/2					-0.19^{d}
							-0.21^{e}
							-0.08^{f}
							-0.15^{g}
2246.900	5s ² 5p ⁶ 6s ² S _{1/2} (<i>F</i> =3)	$5s^25p^66p\ ^2P^o_{1/2}$	7.86E+08	-0.19		-0.19	-0.15^{c}
		-/-					-0.19^{d}
							-0.21^{e}
							-0.08^{f}
							-0.15 ^g

Table C.1: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in Pr V.

^a Kaufman and Sugar (1967)

- ^b Transition probabilities (gA) calculated with HFR method and oscillator strengths $(\log(gf))$ calculated using HFR, MCDHF and AMBiT methods (this work)
- ^c Migdalek and Baylis (1979)
- ^d Migdalek and Wyrozumska (1987)
- ^e Savukov et al. (2003)
- ^f Zilitis (2014)
- ^g Karacoban and Dogan (2015)

Appendix D

Comparison of the radiative parameters for Nd V

$(\hat{\mathbf{A}})a$		ansition	~ 1 4	$\frac{1}{\log(cf)}$	
Λ_{obs} (A) ^a	Lower level	IIIsuuuii Unner level	gA (Previous ^a	(S)	$\log(g_f)$ HFR ^b
370.698	$5s^25p^64f^2$ 5743.4 (J=6)	$5s^25p^54f^25d 275504 9 (J=5)^{\circ}$	4.19E+11	1.09E+11	0.30
371.855	$5s^25p^64f^2$ 2834.3 (J=5)	$5s^25p^54f^25d 271756.6 (J=4)^{\circ}$	1.80E+11	4.02E+09	-1.11
372.550	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 276205.0 (J=2)^{\circ}$	3.78E+11	9.70E+10	1.05
372.828	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 276531.3 (J=4)^o$	6.42E+11	4.77E+07	-2.98
373.070	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^54f^25d 275831.0 (J=3)^o$	4.91E+11	6.10E+10	1.06
373.564	5s ² 5p ⁶ 4f ² 5893.8 (<i>J</i> =2)	5s ² 5p ⁵ 4f ² 5d 273585.8 (<i>J</i> =3) ^o	4.22E+11	3.18E+08	-2.22
373.819	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 273256.0 (<i>J</i> =5) ^o	1.03E+12	1.23E+12	1.36
374.261	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 275504.9 (<i>J</i> =5) ^o	8.80E+11	2.35E+11	0.64
374.390	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 293189.0 (J=7)^o$	1.86E+12	3.64E+08	-2.19
374.658	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 274695.0 (J=4)^o$	9.85E+11	8.36E+11	1.19
374.930	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^34f^25d 278986.5 (J=4)^o$	1.06E+12	2.00E+09	-1.41
375.151	$5s^25p^64t^2$ 7/84.8 (J=3)	$5s^25p^34t^25d 274344.0 (J=3)^6$	1.64E+11	4.68E+08	-1.53
375.451	$5s^25p^64I^2 = 0.0 (J=4)$	$5s^2 5p^6 4I^2 5d 266346.0 (J=5)^6$	1.32E+12	1.4/E+12 1.72E+12	1.44
375.641	$5s^{2}5p^{6}4f^{2}$ 5742 $A(J=5)$	$5s^{2}5p^{5}4l^{2}5d 271055 0 (J=0)^{2}$	1.3/E+12 1.79E+12	1./3E+12 2.00E+12	1.51
375.041	$5s^{2}5p^{6}4f^{2}$ 2834 3 (<i>J</i> =5)	$5s^{2}5p^{5}4l^{2}5d^{2}68468^{0}(J=1)$	1.70E+12 7.01E+11	2.00E+12 2.22E+06	-4.40
377.058	$5s^{2}5p^{6}4f^{2}57434(I-6)$	$5s^{2}5p^{5}4f^{2}5d 270954 6 (J-6)^{\circ}$	$1.59E \pm 12$	1.71E+12	1 51
377.432	$5s^{2}5p^{6}4f^{2} 8311.4 (J=4)$	$5s^{2}5p^{5}4f^{2}5d 273256.0 (J=5)^{\circ}$	3.94E+11	1.59E+11	0.48
408.012	$5s^25p^64f^2 8311.4 (J=4)$	$5s^25p^54f^25d 253402.8 (J=5)^{\circ}$	6.87E+09	6.27E+06	-3.85
412.657	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 245165.8 (J=6)^{\circ}$	2.48E+09	7.70E+08	-1.73
412.734	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 248026.8 (J=7)^o$	1.67E+09	4.86E+09	-0.82
413.770	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 241677.8 (J=3)^o$	1.16E+09	4.17E+07	-3.00
417.562	5s ² 5p ⁶ 4f ² 0.0 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 239482.1 (<i>J</i> =3) ^o	3.24E+09	1.92E+08	-2.33
420.851	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 243355.7 (<i>J</i> =7) ^o	1.43E+10	1.36E+10	-0.45
421.607	5s ² 5p ⁶ 4f ² 0.0 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 237184.8 (<i>J</i> =3) ^o	1.60E+09	3.67E+09	-1.10
424.125	$5s^25p^64f^2$ 5893.8 (<i>J</i> =2)	$5s^25p^54f^25d \ 241677.8 \ (J=3)^o$	2.98E+09	8.89E+11	1.22
427.543	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 241677.8 (J=3)^o$	2.11E+09	2.84E+09	-1.27
427.680	$5s^25p^64f^2 = 0.0 (J=4)$	$5s^25p^54f^25d 233817.4 (J=3)^o$	3.28E+09	6.65E+09	-0.71
428.117	$5s^25p^64t^2 0.0 (J=4)$	$5s^25p^34t^25d 233581.0 (J=5)^6$	5.62E+09	1.54E+09	-1.37
429.107	$5s^25p^64f^25/43.4 (J=6)$	$5s^2 5p^6 4f^2 5d 238/8/.0 (J=1)^6$ $5s^2 5p^5 4f^2 5d 238204.8 (J=2)^6$	1.21E+09	2.32E+07	-3.20
430.290	$5s^{2}5p^{6}4f^{2}$ 5895.8 (J=2)	$5s^{2}5p^{5}4l^{2}5d$ 238294.8 $(J=3)^{2}$	3.43E+08	5.88E+08	-2.01
431 594	$5s^{2}5p^{6}4f^{2}$ 7784 8 (<i>I</i> -3)	$5s^{2}5p^{4}1^{5}3d^{2}230127.0(J=2)$ $5s^{2}5p^{5}4f^{2}5d^{2}394821(J=3)^{o}$	1.912+09 1.25E+09	2.00E+07 2.12E+07	-2.81
432,356	$5s^{2}5p^{6}4f^{2} = 0.0 (J=4)$	$5s^{2}5p^{5}4f^{2}5d^{2}31296^{1}(J=4)^{\circ}$	3 88E+09	5.82E+09	-0.75
432.356	$5s^25p^64f^2$ 5893.8 (J=2)	$5s^25p^54f^25d 237184.8 (J=3)^{\circ}$	3.18E+09	8.14E+06	-3.59
432.389	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 234105.4 (J=5)^o$	1.65E+09	2.51E+09	-1.13
432.448	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 231240.8 (J=4)^{\circ}$	8.12E+08	3.02E+08	-2.13
432.577	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 239482.1 (J=3)^o$	9.20E+08	8.96E+08	-1.62
432.810	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 231046.4 (J=3)^o$	1.52E+09	1.10E+09	-1.52
432.960	5s ² 5p ⁶ 4f ² 0.0 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 230967.9 (<i>J</i> =5) ^o	8.52E+09	3.21E+06	-4.05
433.130	5s ² 5p ⁶ 4f ² 7784.8 (<i>J</i> =3)	5s ² 5p ⁵ 4f ² 5d 238661.2 (<i>J</i> =4) ^o	3.32E+09	1.54E+09	-1.32
433.130	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 239188.9 (J=3)^o$	3.16E+09	1.97E+08	-2.29
433.366	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 233581.0 (J=5)^o$	3.25E+09	1.65E+08	-2.33
433.820	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 238294.8 (J=3)^o$	4.08E+08	5.84E+08	-1.82
434.131	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^34f^25d 238127.6 (J=2)^{o}$	2.45E+09	1.83E+09	-1.31
434.350	$5s^25p^64f^2 5/43.4 (J=6)$	$5s^25p^54f^25d 235965.1 (J=5)^6$	6.99E+08	4.40E+08	-1.87
434.808	$5s^25p^64f^2$ 8311.4 (J=4) $5s^25p^64f^2$ 26088 1 (J=6)	$5s^{2}5p^{6}4I^{2}5d 238294.8 (J=3)^{6}$	7.51E+08	5.19E+08	-1.88
430.840	$5s^{2}5p^{6}4f^{2} = 20088.1 (J=0)$ $5s^{2}5p^{6}4f^{2} = 0.0 (J=4)$	$5s^{2}5p^{5}4f^{2}5d 228737 2 (I-4)^{9}$	5.60E+10	9.0/E+08	-1.49
437.100	$5s \ 5p \ 4l^{\circ} \ 0.0 \ (J=4)$ $5s^{2} 5p^{6} 4f^{2} \ 0.0 \ (J=4)$	5s 5p 41 5d 228757.2 (J=4) $5s^25n^54f^25d 228623 7 (J-5)^{\circ}$	$1.53E\pm00$	1.00E+09	-1.09
437 711	$5s^{2}5n^{6}4f^{2}$ 2834 3 ($I=5$)	$5s^{2}5p^{5}4f^{2}5d^{2}312961(J=4)^{o}$	1.55E+09 1 15E+08	1.25E+09	-2.23
437.812	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 231240.8 (J=4)^\circ$	8.62E+09	3.72E+08	-1.97
437.897	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 234105.4 (J=5)^{\circ}$	4.79E+09	2.86E+09	-1.06
438.228	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 228189.8 (J=3)^o$	5.54E+09	1.10E+09	-1.52
438.228	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 233935.4 (J=7)^o$	1.01E+10	8.47E+08	-1.60
438.430	$5s^25p^64f^2$ 5893.8 (J=2)	$5s^25p^54f^25d 233979.7 (J=2)^o$	3.75E+08	4.34E+08	-1.92
438.742	5s ² 5p ⁶ 4f ² 5893.8 (<i>J</i> =2)	5s ² 5p ⁵ 4f ² 5d 233817.4 (<i>J</i> =3) ^o	5.89E+09	8.00E+08	-1.64
438.913	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 233581.0 (<i>J</i> =5) ^o	2.45E+09	2.45E+09	-1.15
439.265	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 235965.1 (J=5)^o$	2.68E+09	4.66E+08	-1.83
439.918	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 253402.8 (J=5)^o$	2.05E+10	9.61E+09	-0.61
440.129	5s ² 5p ⁶ 4f ² 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 239482.1 (J=3)^o$	3.19E+09	2.96E+09	-1.08

Table D.1: Transition probabilities (gA) and oscillator strengths (log(gf)) for experimentally observed lines in Nd V.

λ_{aba} (Å) ^a	Tr	ansition	aA	$\log(af)$	
1008 (11)	Lower level	Unner level	Previous ^a	HFR ^b	HFR ^b
440 424	$5s^25p^64f^2 0 0 (I-4)$	$\frac{5 s^2 5 p^5 4 f^2 5 d}{5 s^2 5 p^5 4 f^2 5 d} \frac{227051}{227051} 0 (I-3)^{\circ}$	$3.84E\pm00$	3.06E±08	1.03
440.424	5s 3p 41 0.0 (J=4) $5c^2 5r^6 4f^2 12260 7 (J=4)$	$5^{2}5^{5}5^{4}f^{2}5^{4}f^{2}5^{4}f^{2}5^{6$	1.70E+09	3.90E+00	-1.95
440.083	$58 3p^{4}41 12209.7 (J=4)$	$58 \text{ Jp}^{-41} \text{ Ju} 239188.9 (J=3)$	1.79E+09	2.90E+09	-1.00
441.124	$5s^{2}5p^{2}4l^{2} 2834.3 (J=5)$	$5s^{2}5p^{6}4l^{2}5d 229533.7 (J=4)^{6}$	2.28E+09	1.06E+09	-1.42
441.268	$5s^25p^64t^2 0.0 (J=4)$	$5s^25p^34t^25d$ 226618.2 (J=5) ⁶	1.22E+10	2.16E+09	-1.21
441.679	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^34f^25d 226411.4 (J=5)^o$	2.24E+07	3.40E+08	-2.02
441.714	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 238661.2 (J=4)^o$	1.16E+10	6.44E+08	-1.72
441.876	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 252396.0 (J=7)^o$	2.64E+10	4.15E+10	0.06
442.097	5s ² 5p ⁶ 4f ² 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d \ 233979.7 \ (J=2)^o$	1.08E+09	1.44E+08	-2.39
442.216	5s ² 5p ⁶ 4f ² 0.0 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 226134.9 (<i>J</i> =3) ^o	2.88E+08	3.83E+08	-1.99
442.424	5s ² 5p ⁶ 4f ² 7784.8 (<i>J</i> =3)	5s ² 5p ⁵ 4f ² 5d 233817.4 (<i>J</i> =3) ^o	7.09E+09	1.35E+09	-1.41
442.424	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 238294.8 (<i>J</i> =3) ^o	7.25E+09	7.96E+07	-2.68
442.678	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 228737.2 (J=4)^o$	3.99E+09	3.25E+09	-1.04
442.878	$5s^25p^64f^2$ 2834.3 (J=5)	$5s^25p^54f^25d 228623.7 (J=5)^{\circ}$	1.53E+09	3.31E+08	-2.03
442.878	$5s^25p^64f^2$ 8311.4 (J=4)	$5s^{2}5p^{5}4f^{2}5d 234105.4 (J=5)^{\circ}$	1.10E+09	1.54E+09	-1.32
443.066	$5s^25p^64f^2$ 5893.8 (J=2)	$5s^25p^54f^25d 231592.0 (J=3)^{\circ}$	1.29E+09	4.09E+08	-1.95
443 333	$5s^25p^64f^2$ 2834 3 (<i>I</i> =5)	$5s^2 5n^5 4f^2 5d 228398 8 (J=6)^{\circ}$	2 96E+09	8 57E+09	-0.58
444 621	$5s^2 5p^6 4f^2$ 12269 7 (<i>I</i> -4)	$5s^2 5p^5 Af^2 5d 227184 8 (J-3)^{\circ}$	1.03E±00	1.15E±09	-1.52
445 375	$5s^{2}5p^{6}4f^{2} 0 0 (I-4)$	$5s^{2}5p^{5}4f^{2}5d^{2}24520^{3}(J-4)^{9}$	3.22E+00	5.02E±08	1.92
445.575	5s 3p 41 0.0 (J-4) $5c^2 5r^6 4f^2 2824 3 (J-5)$	$5^{2}5^{5}4^{2}5^{4}2^{2}5^{4}2^{2}6^{2}5^{5}4^{2}5^{4}2^{2}6^{2}5^{5}4^{2}5^{4}2^{2}6^{2}5^{5}4^{2}5^{4}2^{2}6^{2}5^{4}2^{2}5^{4}5^{2}5^{2}5^{2}5^{2}5^{2}5^{2}5^{2}5^{2$	3.22E+09	3.02E+08	-1.04
440.833	$58^{-}59^{+}41^{-}2854.5(J=5)$	$58^{-}59^{-}41^{-}50.226018.2(J=3)^{-}$	3.70E+09	2.39E+09	-1.11
447.040	$5s^{2}5p^{4}1^{2} 12269.7 (J=4)$	$5s^{2}5p^{6}4l^{2}5d 235965.1 (J=5)^{6}$	3.04E+09	2.11E+08	-2.10
447.401	$5s^25p^64t^2$ //84.8 (J=3)	$5s^25p^64t^25d 231296.1 (J=4)^6$	3.54E+08	3.93E+08	-1.89
447.514	$5s^25p^64t^2$ 7/84.8 (J=3)	$5s^25p^34t^25d\ 231240.8\ (J=4)^6$	2.51E+09	2.25E+09	-1.17
447.875	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 231592.0 (J=3)^o$	2.21E+09	1.97E+08	-2.29
447.920	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d$ 223252.7 (<i>J</i> =3)°	4.92E+08	6.49E+08	-1.70
448.450	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d \ 231296.1 \ (J=4)^o$	2.62E+09	6.03E+09	-0.77
448.572	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 231240.8 (<i>J</i> =4) ^o	2.68E+09	3.00E+08	-2.05
448.671	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 228623.7 (J=5)^o$	1.93E+10	8.51E+09	-0.61
448.967	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 231046.4 (<i>J</i> =3) ^o	1.81E+09	1.34E+10	-0.39
449.123	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 228398.8 (<i>J</i> =6) ^o	5.63E+09	8.33E+08	-1.61
449.123	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 230967.9 (J=5)^o$	2.48E+09	3.83E+08	-1.90
449.506	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 222466.9 (J=4)^o$	1.59E+09	2.57E+08	-2.11
449.845	$5s^25p^64f^2$ 5893.8 (J=2)	$5s^25p^54f^25d 228189.8 (J=3)^o$	4.01E+09	1.54E+09	-1.35
450.322	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 222061.2 (J=5)^{\circ}$	1.08E+09	7.72E+07	-2.72
450.580	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d$ 248026.8 (J=7)°	1.55E+10	4.86E+09	-0.82
450 781	$5s^25p^64f^2$ 12269 7 (<i>J</i> =4)	$5s^25p^54f^25d 234105 4 (J=5)^{\circ}$	5 67E+07	5 01E+08	-1 79
450.968	$5s^25p^64f^2$ 7784 8 ($I-3$)	$5s^2 5p^5 4f^2 5d 229 1105.1 (J=4)^{\circ}$	2 70E+09	1.07E+08	-2 53
451 077	$5s^25p^64f^2$ 2834 3 (<i>I</i> =5)	$5s^{2}5p^{5}4f^{2}5d^{2}24529^{3}(J-4)^{o}$	2.70E109	1.07E+00	-1.50
451 217	$5s^{2}5p^{6}4f^{2}$ 2834 3 (J=5)	$5s^{2}5p^{-5}4f^{2}5d^{-2}24461^{-6}(J-6)^{0}$	2.41E+09	5.47E+08	1.50
451.217	$5s^{2}5p^{6}4f^{2}$ 12260 7 (<i>I</i> -4)	$5s^{2}5p^{5}4f^{2}5d^{2}224401.0(J=0)$	2.112 ± 00	2.47E+08	2 50
451.571	58 5p 41 12209.7 (J=4)	58 Sp 41 Su 255817.4 (J=3)	1.12E+09	6.03E+07	-2.39
451.040	$5s^{-}5p^{+}41^{-}0.0(J=4)$	$5s^{-}5p^{+}4l^{-}5d 22l^{+}16.7 (J=3)^{-}$	2.02E+08	4.91E+08	-1.85
451.858	$5s^25p^64t^2$ 12269./ (J=4)	$5s^25p^64t^25d 233581.0 (J=5)^6$	2.20E+10	5./9E+09	-0.79
452.015	$5s^25p^64t^2$ 8311.4 (<i>J</i> =4)	$5s^25p^34t^25d 229533.7 (J=4)^{\circ}$	8.67E+09	2.65E+08	-2.13
452.228	$5s^25p^64t^2$ 20551.4 (<i>J</i> =2)	$5s^25p^34t^25d 241677.8 (J=3)^6$	1.18E+09	1.83E+08	-2.24
452.406	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^34f^25d$ 221040.4 (J=3) ^o	1.65E+10	3.10E+07	-3.00
452.524	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d$ 229292.9 (<i>J</i> =5)°	1.32E+10	7.46E+09	-0.65
452.600	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 228737.2 (J=4)^o$	4.21E+09	4.08E+08	-1.92
452.744	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d \ 226618.2 \ (J=5)^o$	5.27E+09	1.13E+09	-1.47
452.881	5s ² 5p ⁶ 4f ² 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 223644.5 (J=6)^o$	4.51E+09	5.47E+08	-1.81
452.991	$5s^25p^64f^2$ 0.0 (<i>J</i> =4)	$5s^25p^54f^25d 220754.5 (J=4)^o$	4.74E+08	1.32E+08	-2.45
453.176	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 226411.4 (J=5)^o$	2.40E+09	5.34E+08	-1.80
453.176	$5s^25p^64f^2$ 5743.4 (J=6)	$5s^25p^54f^25d 226271.3 (J=7)^o$	4.60E+10	2.05E+10	-0.21
453.562	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 220472.9 (J=5)^o$	5.78E+07	1.73E+09	-1.28
453.659	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d$ 228737 2 (<i>I</i> =4)°	6.99E+08	6.58E+08	-1.73
453 914	$5s^25n^64f^2$ 8311 4 (<i>J</i> =4)	$5s^25n^54f^25d$ 228623 7 ($I-5$)°	6.13E+08	2.77E+09	-1.08
454 053	$5s^25n^64f^2$ 2834 3 ($I-5$)	$5s^25p^54f^25d$ 223069 0 ($I-4$)°	6 70F+00	$1.45F \pm 00$	-1 37
454 053	$5s^{2}5n^{6}4f^{2}$ 5803 8 (<i>I</i> -2)	$5s^2 5p^5 4f^2 5d 225007.0 (J=4)$	2 27EL00	8 79F±09	-1.60
454 700 154 700	$5s^{2}5n^{6}Af^{2}57A3A(J-6)$	$5_{\rm s}^{2} 5_{\rm p}^{-5} I f^{2} 5_{\rm d}^{-3} 225137.5 (J-3)$	4.76E+00	6 18E 07	-1.00
454.702	$5s^2 5n^6 Af^2 224 2 (I=0)$	$5_{s}^{2}5_{p}^{5}4f^{2}5_{4}^{2}227164(I=5)^{0}$	4.70E+09	6 82E + 00	-2.09
4,171	Jo JP +1 2034.3 (J=J)	Jo Jp HI JU 222/10.4 (J=J)	+. <i>21</i> 5+09	0.0315+09	-0.00

$\lambda = (\mathring{\lambda})^a$	Tre	ansition	a A (s	$\log(af)$	
Λ_{obs} (A)	L ower level	Lupper level	gravious ^a		ued_b
455 104	$\frac{1}{5a^25\pi^64f^2} = 0.0(1.4)$	$\frac{0}{5c^2 5\pi^5 4f^2 5d} 2106857(1-4)g}$		1 42E+10	0.27
455.194	$58^{-}59^{-}41^{-}0.0(J=4)$	$5s^{-}5p^{+}41^{-}5d\ 219085.7\ (J=4)^{-}$	2.91E+09	1.42E+10	-0.37
455.194	$58^{-}59^{-}41^{-}5895.8(J=2)$	$5s^{-}5p^{+}41^{-}5d\ 2255\ 76.7\ (J=5)^{-}$	0.10E+09	2.74E+09	-1.08
455.318	$5s^25p^64I^2$ 2834.3 (J=5)	$5s^{2}5p^{6}4I^{2}5d 222466.9 (J=4)^{6}$	8.2/E+08	7.02E+08	-1./1
455.954	$5s^25p^64t^2$ 12269.7 (J=4)	$5s^2 5p^3 4t^2 5d 231592.0 (J=3)^3$	1.13E+09	1.02E+09	-1.53
456.059	$5s^25p^64t^2$ 7/84.8 (J=3)	$5s^25p^34t^25d 227051.0 (J=3)^6$	2.77E+09	1.47E+09	-1.53
456.398	$5s^25p^64t^2 0.0 (J=4)$	$5s^25p^34f^25d 219103.5 (J=5)^6$	1.40E+10	4.29E+09	-0.89
456.460	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 245165.8 (J=6)^o$	9.23E+09	5.04E+09	-0.81
456.575	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 231296.1 (J=4)^o$	1.08E+09	6.18E+08	-1.72
456.688	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 231240.8 (J=4)^o$	7.24E+08	5.64E+08	-1.75
456.765	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^54f^25d 239482.1 (J=3)^o$	2.57E+08	1.03E+09	-1.48
457.171	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 227051.0 (J=3)^o$	2.80E+09	1.76E+08	-2.25
457.212	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 224461.6 (J=6)^o$	2.67E+10	5.20E+08	-1.82
457.380	5s ² 5p ⁶ 4f ² 0.0 (<i>J</i> =4)	$5s^25p^54f^25d \ 218638.7 \ (J=5)^o$	1.97E+08	1.73E+09	-1.28
457.380	5s ² 5p ⁶ 4f ² 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 221468.6 (J=6)^o$	1.27E+09	1.28E+09	-1.41
457.380	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	5s ² 5p ⁵ 4f ² 5d 239188.9 (<i>J</i> =3) ^o	8.40E+08	1.39E+08	-2.45
457.939	5s ² 5p ⁶ 4f ² 0.0 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 218371.0 (<i>J</i> =4) ^o	4.76E+09	3.34E+08	-2.02
458.099	5s ² 5p ⁶ 4f ² 5893.8 (<i>J</i> =2)	5s ² 5p ⁵ 4f ² 5d 224181.2 (<i>J</i> =2) ^o	7.18E+08	1.76E+08	-2.27
458.498	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 226411.4 (<i>J</i> =5) ^o	3.39E+09	2.35E+09	-1.14
458.674	$5s^25p^64f^2$ 5893.8 (<i>J</i> =2)	$5s^25p^54f^25d 223914.6 (J=3)^o$	6.30E+09	1.21E+08	-2.49
458.885	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 217916.4 (J=4)^o$	1.47E+10	1.10E+09	-1.47
458.885	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 220754.5 (J=4)^o$	1.83E+09	7.02E+08	-1.71
458.921	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d 223644.5 (J=6)^o$	1.06E+10	5.20E+08	-1.82
459.087	$5s^25p^64f^2$ 8311.4 (J=4)	$5s^25p^54f^25d 226134.9 (J=3)^o$	5.39E+09	5.87E+08	-1.77
459.157	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^54f^25d 225576.7 (J=3)^o$	7.95E+08	2.04E+09	-1.22
459.461	$5s^25p^64f^2$ 2834.3 (J=5)	$5s^25p^54f^25d 220472.9 (J=5)^{\circ}$	2.06E+10	3.17E+09	-1.00
459.606	$5s^25p^64f^2$ 20551.4 (J=2)	$5s^25p^54f^25d 238127.6 (J=2)^{\circ}$	1.92E+09	3.06E+08	-2.03
460.074	$5s^25p^64f^2$ 5893.8 (J=2)	$5s^25p^54f^25d 223252.7 (J=3)^{\circ}$	3.29E+09	2.27E+09	-1.16
460.074	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d$ 225668.8 ($J=5$)°	1.67E+09	1.50E+08	-2.29
460.106	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d 217341.6 (J=4)^{\circ}$	5.52E+09	4.41E+08	-1.92
460 267	$5s^25p^64f^2$ 8311 4 (<i>J</i> =4)	$5s^25n^54f^25d$ 225576 7 ($J=3$)°	7 72E+08	7 56E+08	-1.65
460 267	$5s^25p^64f^2$ 26088 1 (<i>I</i> =6)	$5s^2 5p^5 4f^2 5d 243355 7 (J=7)^{\circ}$	7.42E+00	5.42E+08	-1.80
460 783	$5s^2 5p^6 4f^2$ 12269 7 (<i>I</i> =4)	$5s^2 5p^5 4f^2 5d 2292929 (J=5)^{\circ}$	4 55E+09	2 41E+09	-1.13
460 898	$5s^25p^64f^2$ 5743 4 (<i>I</i> -6)	$5s^2 5p^5 4f^2 5d 2227216 4 (I-5)^{\circ}$	2 52E+09	1.35E+08	-2.42
461 089	$5s^25p^64f^2$ 5893 8 ($I-2$)	5^{3} 5p +1 5d 222710.+ (3=5) 5^{2} 5n ⁵ 4f ² 5d 222773 5 (1=2) ^o	7.86E+08	1.55E+00 1.76E+08	_2.42
461 152	$5s^25p^64f^2$ 2834 3 (<i>I</i> =5)	5^{3} 5p +1 5d 222775.5 (3-2) 5^{2} 5n ⁵ /4f ² 5d 219685 7 (1-4) ^o	1.62E+00	6.86E±08	-1.67
461 366	$5s^{2}5p^{6}Af^{2}$ 7784 8 ($I=3$)	$5s^{2}5p^{5}4f^{2}5d^{2}24529^{3}(J-4)^{o}$	5.60E±09	1.53E±00	-1.07
461.605	$5s^{2}5p^{6}4f^{2}$ 20551 $A(I-2)$	$5s^{2}5p^{5}4f^{2}5d^{2}271848(J-3)^{0}$	9.00L+09	$3.72E\pm00$	0.08
461.803	$5s^{2}5p^{6}4f^{2} 0 0 (I-4)$	$5s^{2}5p^{5}4f^{2}5d^{2}16400^{5}(J=5)^{0}$	7.64E+09	3.72E+09	-0.96
401.095	$5s^{2}5p^{6}4f^{2}77848(I-3)$	5s 5p 41 5d 210499.5 (J=5) $5s^2 5p^5 4f^2 5d 224181 2 (J=2)^{\circ}$	1.04E+09	2.19E+09	-1.10
402.118	5s 3p 41 7784.8 (J-3) $5c^2 5r^6 4f^2 12260 7 (J-4)$	58 Sp 41 Su 224181.2 (J-2) $50^{2} 5n^{5} 4f^{2} 5d 228622 7 (J-5)^{9}$	1.23E+09	$1.92E \pm 00$	-2.22
402.199	$5s^{2}5p^{6}4f^{2}57434(I-6)$	5s 5p 41 5d 228025.7 (J=5) $5s^2 5p^5 4f^2 5d 222061 2 (J=5)^{\circ}$	1.33E+09	1.1/E+09	-0.94
402.270	5s 3p 41 3743.4 (J=0) $5c^2 5r^6 4f^2 3834 3 (J=5)$	$5^{2}5^{5}4^{1}5^{1}4^{2}5^{1}4^{2}5^{1}6^{1}6^{2}5^{1}6^{1}6^{2}5^{1}6^{1}6^{2}5^{1}6^{1}6^{1}6^{1}6^{1}6^{1}6^{1}6^{1}6$	3.74E+0.0	1.14E+00	-2.52
402.387	$58 5p^{-41} 2834.5 (J=3)$	$58 \text{ Sp}^{-41} \text{ Sd} 219105.5 (J=5)$ $5c^2 5r^5 4f^2 5d 229190.8 (J=2)^9$	3.78E+09	1.42E+09	-1.55
403.138	$58 3p^{-41} 12209.7 (J=4)$	$58 \text{ Sp}^{-41} \text{ Su} \text{ 228189.8} (J=3)$	1.93E+09	3.33E+08	-1./0
403.270	$5s^{-}5p^{+}4l^{-}26088.1(J=6)$	$58^{-}59^{-}41^{-}50,241942.1,(J=6)^{-}$	1.15E+10	2.31E+09	-1.13
463.315	$5s^{2}5p^{2}4l^{2} 0.0 (J=4)$	$5s^{2}5p^{2}4l^{2}5d 2l5828.5 (J=5)^{6}$	2.86E+09	1.25E+09	-1.41
463.375	$5s^25p^64t^2$ 2834.3 (J=5)	$5s^{2}5p^{6}4t^{2}5d 218638.7 (J=5)^{6}$	4.48E+09	3.1/E+09	-1.00
465.554	$5s^{-}5p^{\circ}41^{-}5/43.4 (J=6)$	5^{25} 5^{47} 5	4.14E+09	2.65E+09	-1.08
463.814	$5s^{2}5p^{2}4t^{2} 8311.4 (J=4)$	$5s^{-}5p^{-}4t^{-}5d$ 223914.6 (J=3) ⁰	3.19E+09	1.13E+08	-2.53
463.987	5s ² 5p ⁹ 4t ² 2834.3 (<i>J</i> =5)	$5s^{*}5p^{9}4t^{*}5d 218353.2 (J=6)^{o}$	2.81E+09	1.93E+09	-1.21
463.987	5s ² 5p ⁹ 4t ² 5893.8 (<i>J</i> =2)	$5s^{2}5p^{3}4t^{2}5d$ 221416.7 (<i>J</i> =3) ^o	3.18E+08	9.31E+08	-1.55
464.102	5s ² 5p ^o 4f ² 7784.8 (<i>J</i> =3)	$5s^{2}5p^{5}4f^{2}5d$ 223252.7 (<i>J</i> =3) ^o	2.38E+08	1.93E+08	-2.22
464.128	$5s^25p^{\circ}4f^2 \ 0.0 \ (J=4)$	$5s^25p^94f^25d 215456.7 (J=5)^o$	3.83E+09	2.19E+09	-1.16
464.500	5s ² 5p ^o 4f ² 7784.8 (<i>J</i> =3)	$5s^25p^34f^25d$ 223069.0 (<i>J</i> =4)°	7.56E+09	1.63E+07	-3.30
464.810	5s ² 5p ^o 4f ² 5893.8 (<i>J</i> =2)	$5s^2 5p^5 4f^2 5d 221040.4 (J=3)^o$	6.49E+09	8.86E+08	-1.51
464.944	5s ² 5p ⁶ 4f ² 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 217916.4 (J=4)^o$	7.01E+08	2.14E+09	-1.20

λ_{abe} (Å) ^a	Tra	ansition	aA ($\log(af)$	
	Lower level	Upper level	Previous ^a	HFR ^b	HFR ^b
465 504	$5s^25p^64f^2$ 7784 8 ($I-3$)	$5s^25n^54f^25d$ 222602 3 ($I=3$)°	$1.62E \pm 09$	$1.47E \pm 09$	-1.53
465 506	$5s^25p^64f^2$ 12260 7 (<i>I</i> -4)	$5s^2 5p^5 4f^2 5d 222002.5 (3-5)^9$	1.02E+09	$2.61E\pm00$	1.55
405.590	5s 5p 41 12209.7 (5-4) $5c^25p^64f^2 9211 4 (1-4)$	$5s^{2}5r^{5}4f^{2}5d^{2}227051.0(J=3)$	1.47L+09	2.01E+09	-1.27
403.047	$58^{-}59^{+}41^{-}8511.4(J=4)$	$5s^{-}5p^{+}41^{-}5d 223009.0 (J=4)^{-}$	1.84E+08	3.34E+00	-3.90
465./14	$5s^25p^64f^2 5/43.4 (J=6)$	$5s^25p^54f^25d 2204/2.9 (J=5)^6$	1.89E+09	4.26E+08	-1.86
465.802	$5s^25p^64t^2$ //84.8 (J=3)	$5s^25p^34f^25d 222466.9 (J=4)^6$	9.94E+08	1.55E+08	-2.35
466.074	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d$ 220304.1 (<i>J</i> =6) ^o	1.47E+09	1.17E+09	-1.43
466.189	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d \ 217341.6 \ (J=4)^o$	9.77E+08	2.10E+09	-1.24
466.401	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 222716.4 (J=5)^o$	1.03E+09	3.54E+09	-1.02
466.940	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 222466.9 (J=4)^o$	1.49E+09	2.30E+09	-1.18
466.976	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 226411.4 (<i>J</i> =5) ^o	8.45E+08	5.24E+08	-1.78
467.580	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 226134.9 (J=3)^o$	2.83E+09	9.87E+08	-1.53
467.825	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^54f^25d 221538.1 (J=4)^o$	7.54E+08	1.63E+07	-3.30
467.876	$5s^25p^64f^2$ 0.0 (J=4)	$5s^25p^54f^25d 213738.5 (J=4)^{\circ}$	1.08E+09	2.28E+08	-2.20
468 023	$5s^25p^64f^2$ 2834 3 (J=5)	$5s^25p^54f^25d 216499 5 (J=5)^{\circ}$	2 19E+09	1 07E+09	-1 46
468 101	$5s^2 5p^6 4f^2 7784 8 (I-3)$	$5s^2 5n^5 4f^2 5d 221019915 (0 - 5)^{\circ}$	5.71E+07	5.31E+08	-1 78
468.101	$5s^25p^64f^2 = 0.0(J-4)$	$5s^25p^54f^25d 213453 \cap (J=5)^{\circ}$	1.88E±00	0.28E±08	1.70
468 602	5s 5p 41 0.0 (j - 4) $5c^2 5p^6 4f^2 12260 7 (J - 4)$	$5s^{2}5r^{5}4f^{2}5d^{2}15455.0(J-5)$	1.00 ± 00	$9.28E \pm 08$	-1.57
408.002	$58 5p^{4}41 12209.7 (J=4)$	$58 \text{ Jp}^{-41} \text{ Ju} 223008.8 (J=3)$	1.40E+09	2.02E+08	-2.14
468.921	$5s^{2}5p^{2}4l^{2}$ //84.8 (J=3)	$5s^{2}5p^{5}4l^{2}5122l040.4(J=3)^{5}$	1.44E+09	1.45E+07	-3.28
468.974	$5s^25p^64t^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d$ 221538.1 (<i>J</i> =4) ⁶	4.30E+09	3.54E+06	-3.96
469.504	$5s^25p^64t^2$ 2834.3 (J=5)	$5s^25p^34f^25d 215828.5 (J=5)^6$	6.13E+07	6.51E+08	-1.78
469.552	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d$ 220754.5 (<i>J</i> =4)°	7.25E+08	1.55E+08	-2.35
469.711	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d \ 218638.7 \ (J=5)^o$	8.05E+08	4.40E+08	-1.87
470.071	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d 221040.4 (J=3)^o$	7.30E+06	1.59E+07	-2.42
470.146	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 238787.0 (<i>J</i> =7) ^o	7.78E+08	1.15E+09	-1.42
470.326	5s ² 5p ⁶ 4f ² 2834.3 (<i>J</i> =5)	5s ² 5p ⁵ 4f ² 5d 215456.7 (<i>J</i> =5) ^o	2.28E+09	1.07E+09	-1.46
470.350	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d \ 218353.2 \ (J=6)^o$	7.32E+08	1.17E+09	-1.43
470.405	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^54f^25d 220368.9 (J=3)^{\circ}$	9.91E+08	1.22E+08	-2.44
471.122	$5s^25p^64f^2$ 12269.7 (J=4)	$5s^25p^54f^25d 224529.3 (J=4)^{\circ}$	1.27E+09	1.15E+09	-1.43
471.183	$5s^25p^64f^2$ 25892.9 (J=1)	$5s^25p^54f^25d 238127.6 (J=2)^{\circ}$	9.39E+08	4.08E+08	-2.05
471 353	$5s^25p^64f^2$ 8311 4 (<i>I</i> =4)	$5s^2 5p^5 4f^2 5d 220472.9 (J=5)^{\circ}$	4 26E+08	4 66E+08	-1.83
471 567	$5s^25p^64f^2 83114(I-4)$	$5s^{2}5p^{5}Af^{2}5d^{2}20368^{0}(J=3)^{0}$	2.67E±00	2 79E±08	-2.08
471.007	$5s^{2}5p^{6}4f^{2}77848(I-3)$	$5s^2 5p^5 4f^2 5d 210685 7 (J-4)^o$	5.32E+08	1.00E±07	3.44
471.910	5s 5p 41 7/84.8 (J-3) $5c^2 5p^6 4f^2 0.0 (J-4)$	$5^{2}5^{5}7^{4}1^{5}34^{2}5^{4}211278^{2}3(J-3)^{6}$	3.32E+08	1.09E+07	-3.44
475.509	5s 5p 41 0.0 (J=4)	58 Sp 41 Su 211278.5 (J=5) $5c^2 5r^5 4f^2 5d 2112472 (J=5)^9$	1.03E+00	1.29E+00	-2.51
4/3.38/	$58 5p^{2}41 0.0 (J=4)$	$58 \ 5p^{-41} \ 5d \ 211247.5 \ (J=3)$	1.19E+09	2.90E+09	-1.05
4/3.835	$5s^{2}5p^{2}4l^{2}$ 20551.4 (<i>J</i> =2)	$5s^{2}5p^{2}4l^{2}5d 231592.0 (J=3)^{2}$	2.85E+08	2.41E+08	-2.13
473.969	$5s^25p^64t^2$ 12269.7 (J=4)	$5s^25p^34t^25d 223252.1 (J=3)^3$	8.49E+08	1.30E+08	-2.35
474.111	$5s^25p^64t^2 \ 0.0 \ (J=4)$	$5s^25p^34f^25d \ 210920.2 \ (J=4)^6$	3.85E+08	4.30E+08	-1.85
474.414	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d \ 219103.5 \ (J=5)^o$	1.83E+08	3.83E+08	-1.90
474.861	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 213423.3 (J=6)^o$	1.10E+09	1.68E+09	-1.25
474.861	5s ² 5p ⁶ 4f ² 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d \ 218371.0 \ (J=4)^o$	4.11E+08	1.63E+07	-3.30
474.953	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d \ 210545.7 \ (J=5)^o$	2.60E+08	9.28E+08	-1.57
475.445	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 222602.3 (J=3)^o$	4.63E+08	2.61E+09	-1.27
475.891	5s ² 5p ⁶ 4f ² 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 217916.4 (J=4)^o$	5.74E+08	1.54E+09	-1.32
475.984	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d \ 215828.5 \ (J=5)^o$	5.12E+08	1.38E+08	-2.35
476.683	$5s^25p^64f^2$ 12269.7 (J=4)	$5s^25p^54f^25d 222061.2 (J=5)^o$	9.37E+08	6.24E+08	-1.67
477.870	$5s^25p^64f^2$ 12269.7 (J=4)	$5s^25p^54f^25d 221538.1 (J=4)^{\circ}$	5.66E+08	5.09E+08	-1.79
479 649	$5s^25p^64f^2$ 12269 7 (<i>J</i> =4)	$5s^25p^54f^25d$ 220754 5 (J=4)°	1.04E+08	3 64E+08	-1.96
479.817	$5s^25p^64f^2$ 2834 3 ($I-5$)	$5s^2 5n^5 4f^2 5d 211247 3 (J-5)^{\circ}$	1.01E+00 1.15E+00	6.94E+08	-1.66
480 200	$5s^25p^64f^2$ 12269 7 (<i>I</i> -4)	$5s^{2}5p^{5}4f^{2}5d^{2}204729(J=5)^{o}$	1.19E+07	2 11E±08	-2.16
480.277	$5s^{2}5p^{6}4f^{2} 0 0 (I-4)$	$5s^{2}5p^{5}4f^{2}5d^{2}081438(J-5)^{0}$	5 20E+08	2.11L+00	1.05
480 540	$5s^2 5n^6 4f^2 2824 2(1-5)$	$5_{\rm s}^{2}5_{\rm p}^{5}/f^{2}5_{\rm s}^{2}$ $(J=3)$	3 16E + 00	0.84E+07	2 49
400.309	$5_{0}^{2}5_{0}^{2}6_{4}f^{2}$ 25000 0 (J = 3)	$5_{0}^{2}5_{0}^{5}4f^{2}5d^{2}220707(1-2)^{0}$	J.10E+08	2.04E+U/	-2.40
400.309	$58 \text{ sp}^{-41^{-}} 25892.9 (J=1)$	$58 \text{ sp}^{-41} \text{ so} 2539/9.7 (J=2)^{\circ}$	1.01E+08	0.04E+U/	-2.52
480.740	$5s^{-}5p^{-}4I^{-}26088.1 (J=6)$	$5s^{-}5p^{-}41^{-}5d^{-}234105.4(J=5)^{0}$	1.39E+09	9.01E+09	-0.61
481.122	5s ² 5p ³ 41 ² 26088.1 (<i>J</i> =6)	$5s^{-}5p^{-}41^{-}5d 233935.4 (J=7)^{0}$	1.34E+09	3.36E+09	-0.98
481.435	5s ² 5p ⁶ 4t ² 2834.3 (<i>J</i> =5)	$5s^{2}5p^{3}4t^{2}5d 210545.7 (J=5)^{o}$	2.59E+09	1.58E+08	-2.41
481.435	5s ² 5p ^o 4t ² 5743.4 (<i>J</i> =6)	$5s^{2}5p^{9}4f^{2}5d 213453.0 (J=5)^{o}$	8.60E+08	1.95E+08	-2.22
481.509	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^{2}5p^{5}4f^{2}5d 213423.3 (J=6)^{o}$	5.82E+08	9.80E+08	-1.48
482.119	5s ² 5p ⁶ 4f ² 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 219685.7 (J=4)^o$	7.15E+08	2.23E+08	-2.12
482.741	$5s^25p^64f^2$ 0.0 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 207148.2 (<i>J</i> =5) ^o	2.14E+09	1.07E+08	-2.45

λ_{obs} (Å) ^a	Tra	ansition	qA	$\log(qf)$	
	Lower level	Upper level	Previous ^a	HFR ^b	HFR ^b
482 741	$5s^25p^64f^2$ 8311 4 (<i>J</i> =4)	$5s^25n^54f^25d 215456 7 (J=5)^{\circ}$	8 11E+08	1 55E+07	-3.28
483 474	$5s^2 5p^6 4f^2$ 12269 7 (<i>I</i> -4)	$5s^2 5n^5 4f^2 5d 219103 5 (J-5)^{\circ}$	2 76E+08	1.55E+0.08	-2 33
484 244	$5s^25p^64f^2 0 0 (I-4)$	$5s^2 5p^5 4f^2 5d 206509 1 (J-5)^{\circ}$	6.46E±08	2 13E±08	2.55 2.14
404.244	5s 5p 41 0.0 (j - 4) $5c^2 5p^6 4f^2 12260 7 (J - 4)$	$5s^{2}5r^{5}4f^{2}5d^{2}196397(J=5)$	0.40E+08	2.13E+08	-2.14
404.377	$58 3p^{-41} 12209.7 (J=4)$	$58 \text{ Sp}^{-41} \text{ Su} \text{ 218058.7} (J=3)$	1.39E+08	$2.11E \pm 00$	-2.10
485.529	$5s^{-}5p^{+}41^{-}7/84.8(J=3)$	$58^{-}59^{-}41^{-}50\ 213738.5\ (J=4)^{-}$	3.70E+08	1.30E+08	-2.54
486.050	$5s^{2}5p^{4}1^{2} 0.0 (J=4)$	$55^{\circ}59^{\circ}41^{\circ}50\ 205744.4\ (J=4)^{\circ}$	2.01E+08	0.19E+07	-2.04
486.795	$5s^{2}5p^{4}I^{2} = 8311.4 (J=4)$	$55^{\circ}59^{\circ}41^{\circ}50\ 213738.5\ (J=4)^{\circ}$	1.32E+08	1.13E+09	-1.4/
486.881	$5s^2 5p^6 4I^2 5893.8 (J=2)$	$5s^{2}5p^{6}4I^{2}5d 2112/8.3 (J=3)^{6}$	2.35E+08	3.28E+08	-1.93
487.468	$5s^25p^64t^2$ 8311.4 (<i>J</i> =4)	$5s^{2}5p^{6}4I^{2}5d 2I3453.0 (J=5)^{6}$	1.36E+09	4.60E+08	-1.84
487.629	$5s^25p^64t^2$ 12269.7 (J=4)	$5s^25p^34t^25d 217341.6 (J=4)^6$	4.85E+08	7.28E+07	-2.57
488.281	$5s^25p^64t^2 5/43.4 (J=6)$	$5s^25p^34t^25d 210545.7 (J=5)^6$	9.57E+07	1.95E+08	-2.22
490.971	$5s^25p^64t^2$ 2834.3 (J=5)	$5s^25p^34t^25d$ 206509.1 (J=5) ⁶	4.98E+08	1.18E+08	-2.40
491.084	$5s^25p^64t^2$ 20551.4 (<i>J</i> =2)	$5s^25p^34t^25d 224181.2 (J=2)^3$	2.21E+08	1.92E+08	-2.16
491.169	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^34f^25d \ 203596.3 \ (J=5)^o$	1.94E+08	2.28E+07	-3.09
491.279	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 215828.5 (J=5)^o$	4.26E+08	1.93E+08	-2.17
491.422	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^54f^25d 211278.3 (J=3)^o$	1.16E+08	1.23E+07	-3.25
491.730	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^54f^25d$ 223914.6 (<i>J</i> =3)°	4.31E+08	1.83E+08	-2.24
492.158	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d \ 215456.7 \ (J=5)^o$	1.23E+08	3.93E+07	-2.86
492.695	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d \ 211278.3 \ (J=3)^o$	4.77E+08	4.76E+07	-2.77
492.769	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d \ 211247.3 \ (J=5)^o$	2.72E+08	4.99E+08	-1.78
492.830	5s ² 5p ⁶ 4f ² 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d \ 205744.4 \ (J=4)^o$	2.18E+09	3.50E+08	-1.91
493.343	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^54f^25d 223252.7 (J=3)^o$	1.67E+08	5.67E+07	-2.69
493.571	5s ² 5p ⁶ 4f ² 8311.4 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 210920.2 (<i>J</i> =4) ^o	1.40E+08	1.70E+08	-2.23
494.061	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 208143.8 (<i>J</i> =5) ^o	6.28E+08	1.45E+08	-2.33
496.355	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	5s ² 5p ⁵ 4f ² 5d 213738.5 (<i>J</i> =4) ^o	8.55E+08	5.64E+08	-1.75
496.512	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁵ 4f ² 5d 207148.2 (<i>J</i> =5) ^o	3.53E+08	3.77E+07	-2.87
497.838	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^54f^25d 221416.7 (J=3)^o$	9.50E+07	8.49E+07	-2.51
498.098	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d \ 206509.1 \ (J=5)^o$	5.88E+08	4.68E+08	-1.79
498.232	$5s^25p^64f^2$ 27478.7 (<i>J</i> =2)	$5s^25p^54f^25d 228189.8 (J=3)^o$	1.35E+08	2.62E+08	-2.02
498.685	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 226618.2 (J=5)^o$	2.00E+08	2.38E+07	-3.05
499.177	$5s^25p^64f^2 0.0 (J=4)$	$5s^25p^54f^25d \ 200327.2 \ (J=4)^o$	1.43E+08	3.60E+08	-1.89
499.546	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 226271.3 (J=7)^o$	2.34E+08	2.05E+10	-0.21
499.872	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^54f^25d 202884.9 (J=6)^o$	3.65E+08	9.33E+07	-2.47
500.421	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^54f^25d \ 208143.8 \ (J=5)^o$	3.52E+08	4.99E+08	-1.78
502.495	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d 211278.3 (J=3)^{\circ}$	3.73E+08	1.78E+08	-2.17
502.559	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^54f^25d\ 211247.3\ (J=5)^o$	1.89E+08	2.67E+08	-2.01
503.093	$5s^25p^64f^2$ 2834.3 (J=5)	$5s^25p^54f^25d \ 201606.0 \ (J=5)^o$	2.62E+08	2.59E+09	-1.11
503.384	$5s^25p^64f^2$ 27478.7 (<i>J</i> =2)	$5s^25p^54f^25d 226134.9 (J=3)^{\circ}$	1.58E+09	3.68E+08	-2.02
504.091	$5s^25p^64f^2$ 26088.1 (<i>J</i> =6)	$5s^25p^54f^25d 224461.6 (J=6)^{\circ}$	8.51E+07	7.80E+08	-1.55
504.547	$5s^25p^64f^2$ 8311.4 (J=4)	$5s^25p^54f^25d \ 206509.1 \ (J=5)^{\circ}$	1.98E+08	6.24E+08	-1.79
505.148	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^54f^25d 205744.4 (J=4)^{\circ}$	1.63E+08	4.79E+06	-3.74
505.425	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d$ 203596.3 (J=5)°	1.25E+09	3.39E+08	-1.89
507.251	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^54f^25d$ 202884.9 (<i>J</i> =6)°	5.01E+08	4.92E+08	-1.72
507.919	$5s^25p^64f^2$ 25892 9 (<i>J</i> =1)	$5s^2 5p^5 4f^2 5d 222773 5 (J=2)^{\circ}$	1.65E+08	6.85E+05	-4 52
508 392	$5s^2 5n^6 4f^2$ 27478 7 (<i>I</i> =2)	$5s^2 5p^5 4f^2 5d 224181 2 (J=2)^{\circ}$	4.19E+08	6.86E+05	-4 52
508 568	$5s^2 5p^6 4f^2$ 26088 1 (<i>I</i> =6)	$5s^2 5p^5 4f^2 5d 222716 4 (I=5)^{\circ}$	2 13E+08	6.08E+06	-3.62
510 267	$5s^25p^64f^2$ 26088 1 (<i>J</i> =6)	$5s^{2}5p^{5}4f^{2}5d^{2}22061^{2}(I-5)^{\circ}$	5 20E±08	1.21E±08	_2 32
513 634	$5s^{2}5p^{6}4f^{2}$ 5803 8 ($I-2$)	$5s^{2}5p^{5}4f^{2}5d 200585 8 (J-3)^{\circ}$	1.02E+08	0.04E±06	3.43
514 828	$5s^{2}5p^{6}4f^{2}$ 12260 7 (<i>I</i> -4)	$5s^{2}5p^{5}4f^{2}5d^{2}00585.8(J=5)^{0}$	$1.92E \pm 08$	9.04E+00	-5.45
514.020	5s 3p 41 12209.7 (J-4) $5c^2 5r^6 4f^2 26088 1 (J-6)$	$5^{2}5^{2}5^{5}4f^{2}5d$ 2200309.1 (J=5)	1.09E+08	1.56E+07	-2.01
J14.00/ 515 204	$5s^{2}5n^{6}Af^{2}$ 7784 8 ($I=0$)	$5_{s}^{2}5_{p}^{5}4f^{2}5_{4}^{2}019295(I_{-4})^{0}$	J.7JE+U0 1 07E+00	1.JUE+U0	-2.10 1.07
516.056	$J_{5} J_{5} J_{7} J_{7$	$5_{0}^{2}5_{0}^{5}4_{1}^{2}5_{4}^{1}100672.6(J-1)^{0}$	1.0/E+08	2.72E+U8	-1.9/
516.000	$J_{5}^{2} S_{7}^{-6} 4f^{2} S_{7}^{-11} 4(J-4)$	58 Sp^{-41} 30 1990/3.0 $(J=1)^{\circ}$	2.29E+08	3.20E+U8	-1.89
510.720	$35^{-}5p^{-}41^{-}8511.4(J=4)$	$55^{2}5^{4}5^{4}5^{4}$	7.00E+07	2.33E+0/	-3.00
510.859	$5s^{-}5p^{-}4I^{-}12269.7 (J=4)$	$55^{2}5^{4}5^{4}5^{1}2005^{6}5^{2}6^{6}(J=4)^{6}$	3.88E+08	7.03E+0/	-2.31
518.668	$5s^{-}5p^{+}4I^{-} / / 84.8 (J=3)$	$5s^{-}5p^{+}41^{-}5d\ 200585.8\ (J=3)^{\circ}$	2.09E+08	8.09E+0/	-2.44
520.115	$5s^{-}5p^{-}4I^{-}26088.1 (J=6)$	$5s^{-}5p^{-}41^{-}5d 218353.2 (J=6)^{0}$	5.26E+08	1.56E+08	-2.18
520.797	$5s^{-}5p^{\circ}41^{-}8311.4(J=4)$	$5s^{-}5p^{\circ}41^{*}5d 200327.2 (J=4)^{\circ}$	9.02E+07	0.95E+07	-2.56
527.512	$5s^{-}5p^{\circ}41^{-}12269.7 (J=4)$	$5s^{-}5p^{-}41^{-}5d$ 201838.5 (J=4) ⁶	/.3/E+0/	1.11E+0/	-3.57
528.159	Ss [*] Sp [×] 41 [*] 12269.7 (J=4)	$3s^{3}5p^{3}41^{3}5d 201606.0 (J=5)^{6}$	1.0/E+08	5.83E+08	-1.72

λ_{obs} (Å) ^a	Tran	sition	gA ($\log(qf)$	
000 ()	Lower level	Upper level	Previous ^a	HFR^{b}	HFR ^b
544.068	$5s^25p^64f^2$ 27478.7 (J=2)	$5s^25p^54f^25d\ 211278.3\ (J=3)^o$	2.58E+08	3.38E+07	-2.81
552 305	$5s^25p^64f^2$ 26088 1 (<i>J</i> =6)	$5s^25n^54f^25d$ 207148 2 ($J=5$)°	1.52E+08	5 76E+06	-3 59
575 433	$5s^2 5p^6 4f^2$ 25892 9 (<i>I</i> -1)	$5s^2 5p^5 4f^2 5d 1996736 (J-1)^{\circ}$	1.32E+0.00 1.27E+0.08	5.76E+00	-2.58
713 801	$5s^{2}5p^{6}4f^{2}$ 2834 3 ($I=5$)	$5s^{2}5p^{6}4f5d 142910 8 (I-5)^{\circ}$	5.00E±06	2.51E±06	-3.68
720.026	$5s^{2}5p^{6}4f^{2}57424(I-6)$	$5s^{2}5p^{6}4f5d 142010.8 (J=5)^{6}$	5.00E+00	2.31E+00	-3.00
729.050	$58 \ 5p^{2}41 \ 5745.4 \ (J=0)$	$58 \text{ Sp}^{-4130} 142910.8 (J=3)^{-5}$	0.20E+07	0.0/E+0/	-2.20
738.999	$55^{-}55^{-}645^{2}$ 9211 4 (1-4)	$55^{-}59^{-}4150155518.5(J=5)^{2}$	3.20E+07	2.83E+07	-2.00
742.942	$5s^{2}5p^{2}4l^{2}$ 8311.4 (<i>J</i> =4)	$5s^{2}5p^{6}415d 142910.8 (J=5)^{6}$	3.20E+07	6.90E+07	-2.21
744.269	$5s^2 5p^6 4f^2 0.0 (J=4)$	$5s^2 5p^6 4f5d 134359.7 (J=4)^6$	2.00E+07	2.91E+07	-2.58
/48.900	$5s^25p^64t^2$ 2834.3 (J=5)	$5s^2 5p^6 4f5d \ 136363.4 \ (J=6)^6$	3.00E+07	4.26E+07	-2.42
754.159	$5s^25p^64f^2 = 0.0 (J=4)$	$5s^2 5p^6 4f5d 132597.5 (J=5)^6$	3.00E+07	4.27E+07	-2.41
756.472	$5s^25p^64t^2$ 2834.3 (J=5)	$5s^25p^64f5d 135027.2 (J=5)^6$	9.80E+07	1.19E+08	-1.95
756.650	$5s^25p^64t^2$ 0.0 (<i>J</i> =4)	$5s^25p^64f5d 132162.1 (J=4)^6$	9.10E+07	1.44E+08	-1.87
758.925	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^64f5d 139549.8 (J=3)^6$	2.40E+07	4.62E+07	-2.36
760.311	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	$5s^25p^64f5d 134359.7 (J=4)^6$	1.42E+08	1.09E+08	-1.99
761.971	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^2 5p^6 4f5d 139549.8 (J=3)^o$	1.80E+07	4.80E+07	-2.34
762.753	$5s^25p^64f^2$ 0.0 (<i>J</i> =4)	$5s^25p^64f5d 131104.7 (J=3)^o$	1.53E+08	1.23E+08	-1.93
765.456	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^64f5d \ 142910.8 \ (J=5)^o$	1.86E+08	1.82E+08	-1.76
765.579	$5s^25p^64f^2$ 5743.4 (<i>J</i> =6)	$5s^25p^64f5d \ 136363.4 \ (J=6)^o$	9.35E+08	1.34E+09	-0.90
765.973	$5s^25p^64f^2$ 0.0 (<i>J</i> =4)	5s ² 5p ⁶ 4f5d 130553.0 (<i>J</i> =4) ^o	2.39E+08	3.88E+08	-1.43
770.635	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	5s ² 5p ⁶ 4f5d 132597.5 (<i>J</i> =5) ^o	7.88E+08	1.14E+09	-0.96
773.230	$5s^25p^64f^2$ 2834.3 (<i>J</i> =5)	5s ² 5p ⁶ 4f5d 132162.1 (<i>J</i> =4) ^o	3.23E+10	4.31E+09	-0.37
773.493	5s ² 5p ⁶ 4f ² 5743.4 (<i>J</i> =6)	5s ² 5p ⁶ 4f5d 135027.2 (<i>J</i> =5) ^o	4.08E+10	5.47E+09	-0.27
774.567	$5s^25p^64f^2$ 0.0 (<i>J</i> =4)	5s ² 5p ⁶ 4f5d 129104.5 (<i>J</i> =3) ^o	2.51E+10	3.48E+09	-0.46
783.863	5s ² 5p ⁶ 4f ² 7784.8 (<i>J</i> =3)	5s ² 5p ⁶ 4f5d 135359.2 (<i>J</i> =2) ^o	9.13E+08	1.14E+09	-0.94
783.912	$5s^25p^64f^2 0.0 (J=4)$	5s ² 5p ⁶ 4f5d 127565.1 (<i>J</i> =4) ^o	4.13E+08	5.32E+08	-1.27
784.105	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	5s ² 5p ⁶ 4f5d 135318.3 (<i>J</i> =3) ^o	8.10E+07	1.39E+08	-1.85
784.483	$5s^25p^64f^2$ 5893.8 (<i>J</i> =2)	5s ² 5p ⁶ 4f5d 133366.3 (<i>J</i> =1) ^o	6.97E+08	9.74E+08	-1.01
785.669	$5s^25p^64f^2$ 12269.7 (<i>J</i> =4)	$5s^25p^64f5d \ 139549.8 \ (J=3)^o$	2.03E+09	2.66E+09	-0.57
787.091	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^64f5d 147601.4 (J=1)^o$	4.66E+08	6.27E+08	-1.18
787.359	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^64f5d \ 135318.3 \ (J=3)^o$	1.74E+09	2.46E+09	-0.60
789.169	$5s^25p^64f^2$ 8311.4 (<i>J</i> =4)	$5s^25p^64f5d \ 135027.2 \ (J=5)^o$	2.60E+08	2.55E+08	-1.58
789.440	$5s^25p^64f^2$ 5893.8 (<i>J</i> =2)	$5s^25p^64f5d \ 132565.8 \ (J=2)^o$	6.80E+07	2.57E+07	-2.58
790.043	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^64f5d 134359.7 (J=4)^o$	3.20E+07	5.62E+07	-2.24
793.348	$5s^25p^64f^2$ 8311.4 (J=4)	$5s^25p^64f5d 134359.7 (J=4)^o$	3.94E+08	2.73E+08	-1.55
798.654	$5s^25p^64f^2$ 5893.8 (J=2)	$5s^25p^64f5d 131104.7 (J=3)^o$	3.90E+07	6.97E+07	-2.13
801.406	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^64f5d 132565.8 (J=2)^o$	2.17E+08	4.07E+08	-1.37
804.005	$5s^25p^64f^2$ 7784.8 (J=3)	$5s^25p^64f5d$ 132162.1 (<i>J</i> =4)°	2.94E+08	3.58E+08	-1.41
810.898	$5s^25p^64f^2$ 7784.8 (<i>J</i> =3)	$5s^25p^64f5d 131104.7 (J=3)^o$	9.94E+08	1.32E+09	-0.84
811.616	$5s^25p^64f^2$ 5893 8 (<i>J</i> =2)	$5s^25n^64f5d$ 129104 5 (J=3)°	2.29E+08	2.66E+08	-1 53
814 378	$5s^2 5p^6 4f^2 83114 (I=4)$	$5s^2 5p^6 4f5 d 131104 7 (I=3)^o$	6.10E+07	1.27E+08	-1.85
814 539	$5s^25n^64f^2$ 7784 8 (<i>I</i> =3)	$5s^2 5p^6 4f5 d 130553 0 (J=4)^{\circ}$	1 30E+07	6 74E+06	-3.13
814 616	$5s^{2}5p^{6}4f^{2}$ 12269 7 (<i>I</i> -4)	$5s^2 5p^6 4f5 d 135027 2 (I-5)^{\circ}$	7.10E+07	2.55E+08	-1.58
815 087	$5s^25p^64f^2$ 25050 6 (<i>I</i> =0)	5^{3} 5p +15d 135027.2 (3-5) 5^{2} 5p ⁶ 4f5d 147601 4 (1-1) ^o	1 90E±07	2.33E+00	-2.51
817 207	$5s^{2}5p^{6}4f5d$ 127565 1 (<i>I</i> -4) ^o	$5s^{2}5p^{6}4f6p^{2}400106(I-4)$	0.57E+08	2.75E+07	0.80
818.060	$5s^{2}5p^{6}4f^{2}$ 8311 $A(I-4)$	$5s^{2}5p^{6}4f5d 130553 0 (J-4)^{\circ}$	4.00E+08	6.27E+09	-0.09
810.000	5s 3p 4i 8311.4 (J = 4) $5s^2 5p^6 4f^2 12260 7 (J = 4)$	5s 5p 415d 130355.0 (J-4) $5s^2 5p^6 4f5d 134250 7 (J-4)^{\circ}$	4.90E+08	1.47E+00	-1.10
821.020	5s 3p 4i 12209.7 (J=4) $5s^2 5p^6 4f^2 5803 8 (J=2)$	5s 5p 415d 134359.7 (J=4) $5s^2 5p^6 4f5d 137558 8 (J=2)^{\circ}$	6.90E+08	0.56E+09	-0.79
821.930	$5s^{-}5p^{+}4l^{-}5895.8(J=2)$	$5s^{-}5p^{-}4130127558.8(J=2)^{2}$	0.31E+08	9.30E+08	-0.97
827.838	$55^{-}5p^{+}41^{-}8511.4(J=4)$	$5s^{2}5p^{2}4130129104.5(J=3)^{2}$	1.90E+07	1.82E+07	-2.08
830.132	$5s^{2}5p^{2}4130131104.7 (J=3)^{2}$	$5s^{-}5p^{*}416p \ 251565.0 \ (J=2)$	0.40E+08	1.00E+08	-1.15
832.481	$5s^{2}5p^{6}4l^{2} = 2/4/8.7 (J=2)$	$5s^{2}5p^{6}415d 147601.4 (J=1)^{6}$	1.25E+08	1.70E+08	-1.69
854.082	$55^{-}5p^{+}41^{-}12269./(J=4)$	$55^{2}57^{4}150 132162.1 (J=4)^{6}$	3.00E+06	8.80E+04	-5.00
834.912	$5s^{*}5p^{*}41^{*}$ //84.8 (J=3)	$5s^{-}5p^{\circ}415d 12/558.8 (J=2)^{0}$	1.30E+07	3.14E+07	-2.44
836.311	$5s^{*}5p^{*}415d 12/558.8 (J=2)^{o}$	5s-5p°4t6p 24/130.7 (<i>J</i> =1)	1.35E+09	1.82E+09	-0.74
838.547	5s*5p°4t ² 8311.4 (<i>J</i> =4)	$5s^{\circ}5p^{\circ}4t5d 127565.1 (J=4)^{o}$	3.22E+08	6.47E+08	-1.12
839.543	$5s^{2}5p^{6}4t5d 127565.1 (J=4)^{o}$	5s ² 5p ⁰ 4f6p 246677.6 (<i>J</i> =4)	4.06E+09	4.97E+09	-0.30
840.350	5s ² 5p ^o 4f ² 20551.4 (<i>J</i> =2)	5s ² 5p ⁶ 4f5d 139549.8 (<i>J</i> =3) ^o	9.80E+07	8.10E+07	-2.00
840.350	5s ² 5p ^o 4f5d 132565.8 (<i>J</i> =2) ^o	5s ² 5p ^o 4f6p 251563.0 (<i>J</i> =2)	2.44E+09	1.99E+09	-0.69
845.426	5s ² 5p ^o 4f ² 12269.7 (<i>J</i> =4)	5s ² 5p ^o 4f5d 130553.0 (<i>J</i> =4) ^o	5.50E+07	7.30E+06	-3.07
848.507	$5s^25p^64f5d 132162.1 (J=4)^o$	5s ² 5p ⁶ 4f6p 250015.7 (<i>J</i> =5)	6.59E+08	7.85E+08	-1.10
849.200	$5s^25p^64f5d 132162.1 (J=4)^o$	5s ² 5p ⁶ 4f6p 249919.6 (<i>J</i> =4)	6.26E+08	2.27E+08	-1.63

$\lambda_{obs} ({ m \AA})^a$	Tran	sition	gA ((s^{-1})	$\log(gf)$
	Lower level	Upper level	Previous ^a	HFR^{b}	HFR^{b}
849.444	5s ² 5p ⁶ 4f ² 20551.4 (<i>J</i> =2)	5s ² 5p ⁶ 4f5d 138275.4 (<i>J</i> =1) ^o	1.18E+08	1.70E+08	-1.68
851.653	5s ² 5p ⁶ 4f5d 132597.5 (<i>J</i> =5) ^o	5s ² 5p ⁶ 4f6p 250015.7 (<i>J</i> =5)	1.44E+09	1.75E+09	-0.74
855.995	5s ² 5p ⁶ 4f ² 26088.1 (<i>J</i> =6)	5s ² 5p ⁶ 4f5d 142910.8 (<i>J</i> =5) ^o	4.36E+09	6.20E+09	-0.11
860.561	$5s^25p^64f5d \ 135359.2 \ (J=2)^o$	$5s^25p^64f6p \ 251563.0 \ (J=2)$	2.34E+09	3.53E+09	-0.42
861.143	$5s^25p^64f5d \ 130553.0 \ (J=4)^o$	$5s^25p^64f6p$ 246677.6 (<i>J</i> =4)	5.48E+08	4.26E+08	-1.34
864.631	$5s^25p^64f5d 134359.7 (J=4)^o$	$5s^25p^64f6p$ 250015.7 (J=5)	9.41E+08	9.52E+08	-0.99
865.353	$5s^25p^64f5d 134359.7 (J=4)^o$	$5s^25p^64f6p$ 249919.6 (<i>J</i> =4)	6.93E+09	7.85E+09	-0.07
866.776	$5s^25p^64f5d 134359.7 (J=4)^o$	5s ² 5p ⁶ 4f6p 249730.1 (<i>J</i> =3)	7.53E+09	8.30E+09	-0.05
867.342	$5s^25p^64f^2$ 12269.7 (J=4)	$5s^25p^64f5d$ 127565.1 (J=4)°	1.06E+08	9.35E+07	-1.93
867.622	$5s^25p^64f5d 131104.7 (J=3)^o$	$5s^25p^64f6p 246362.2 (J=2)$	4.42E+09	4.87E+09	-0.28
868.546	$5s^25p^64f5d 127558.8 (J=2)^o$	$5s^25p^64f6p$ 242694.9 (J=3)	5.40E+07	1.90E+08	-1.69
868.584	$5s^25p^64f5d 127565.1 (J=4)^o$	$5s^25p^64f6p$ 242694.9 (J=3)	6.63E+08	7.17E+08	-1.12
869.650	$5s^25p^64f5d \ 135027.2 \ (J=5)^o$	$5s^25p^64f6p$ 250015.7 (J=5)	6.92E+09	8.37E+09	-0.05
870.381	$5s^25p^64f5d 135027.2 (J=5)^o$	$5s^25p^64f6p$ 249919.6 (<i>J</i> =4)	3.31E+09	3.31E+09	-0.45
871.020	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^64f5d$ 135359.2 (<i>J</i> =2) ^o	6.40E+07	1.58E+08	-1.69
871.333	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^64f5d \ 135318.3 \ (J=3)^o$	2.35E+08	3.28E+08	-1.36
872.339	$5s^25p^64f5d 130553.0 (J=4)^{\circ}$	$5s^25p^64f6p 245187.5 (J=3)$	9.03E+09	1.75E+08	-1.70
872.869	$5s^25p^64f5d 132565.8 (J=2)^o$	$5s^25p^64f6p 247130.7 (J=1)$	1.48E+09	1.55E+09	-0.77
873.241	$5s^25p^64f5d 132162 1 (J=4)^{\circ}$	$5s^25p^64f6p 246677.6 (J=4)$	9.59E+08	1.18E+09	-0.89
874 034	$5s^25p^64f5d 135318 3 (J=3)^{\circ}$	$5s^2 5p^6 4f6p 249730 1 (J=3)$	9 75E+08	8 67E+08	-1.02
874 981	$5s^2 5p^6 4f^2$ 25892 9 (<i>J</i> =1)	$5s^2 5p^6 4f5d 140180 8 (J=2)^{\circ}$	1 78E+08	2.74E+08	-1 44
876 574	$5s^2 5p^6 4f5d 132597 5 (J=5)^{\circ}$	$5s^2 5p^6 4f 6p 246677 6 (J=4)$	9 24E+09	1.10E+10	0.09
878 758	$5s^2 5p^6 4f5d 132565 8 (I=2)^{\circ}$	$5s^2 5n^6 4f6n 246362 2 (I=2)$	3 75E+09	5.00E+09	-0.25
879.009	$5s^2 5p^6 4f5d 133366 3 (J-1)^o$	$5s^2 5p^6 4f6p 247130.7 (I-1)$	2.05E+09	2.60E+09	-0.54
879 876	5° 5p 415d 135360.5 (3=1) 5° 5p ⁶ 4f5d 136363 4 (<i>I</i> =6) ^o	$5s^{2}5p^{6}4f6p^{2}500157(J=5)$	2.05E+09	2.00E+0	0.34
880 359	$5s^{2}5p^{6}4f5d 129104 5 (J-3)^{o}$	$5s^{2}5p^{6}4f6p^{2}250013.7(3=3)$	6.40E+08	2.73E+10	-1 28
883 204	$5s^2 5p^6 4f^2$ 25050 6 (<i>I</i> =0)	$5s^2 5p^6 4f5d 138275 4 (I=1)^{\circ}$	1.42E+08	2 11E+08	-1.55
884 759	$5s^2 5p^6 4f5d 132162 1 (I=4)^{\circ}$	$5s^2 5n^6 4f6n 245187 5 (I=3)$	4 84F+09	7 25E+09	-0.08
884 982	$5s^2 5p^6 4f5d 133366 3 (I=1)^{\circ}$	$5s^2 5p^6 4f6p 246362 2 (I=2)$	1.01E+09 1.19E+08	2 20E+08	-1.60
887 294	$5s^2 5p^6 4f^2 274787 (I=2)$	$5s^2 5p^6 4f5d 140180 8 (I=2)^{\circ}$	8 18F+08	1.12E+09	-0.82
887 899	$5s^{2}5p^{6}4f^{2}$ 25892 9 (<i>I</i> -1)	$5s^{2}5p^{6}4f5d 138519 2 (J-0)^{o}$	2.05E+08	$2.84E \pm 0.8$	-0.02
888 619	$5s^{2}5p^{6}4f5d 130553 0 (I-4)^{\circ}$	$5s^2 5p^6 4f6p 243087 0 (I-4)$	2.05E+00	2.04E+00	-0.60
889 820	$5s^2 5p^6 4f^2 25802.0 (J-1)$	$5s^25p^64f5d 138275 A (I-1)^{\circ}$	1.85E±08	2.20E+09	-0.00
800 320	$5s^{2}5p^{6}4f5d 1343597 (J-4)^{o}$	$5s^25n^64f6n 246677.6 (J-4)$	1.65E+08	1.18F±00	-0.80
801 732	$5s^{2}5p^{6}4f5d 130553 0 (J-4)^{o}$	$5s^{2}5p^{6}4f6p^{2}42694^{6}9(I=3)$	1.04E+09	1.10E+09	-0.89
892 292	$5s^{2}5p^{6}4f^{2}$ 27478 7 ($I-2$)	$5s^{2}5p^{6}4f5d 139549 8 (J-3)^{o}$	2 59E+08	3.74E+08	-1.70
802.272	$5s^{2}5p^{6}4f^{2}$ 20551 $A(I=2)$	$5s^2 5p^6 4f5d 132565 8 (J-2)^o$	5.60E±08	7.83E±08	-0.97
802.743	$5s^{2}5p^{6}4f5d 130540 8 (I-3)^{\circ}$	$5s^{2}5p^{6}4f6p^{2}515630(J-2)$	2.00E+08	3.26E±00	-0.77
802.743	$5s^{2}5p^{6}4f5d 1311047 (I-3)^{o}$	$5s^{2}5p^{6}4f6p^{2}230870(J=4)$	1.21E±09	1.20E+09	-0.45
892.998	$5s^{2}5p^{6}4f5d$ 127558 8 ($I-2$) ^o	$5s^{2}5n^{6}4f6n 2302325 (I-2)$	1.21E+09	1.27E+09 6 35E+00	-0.85
805 662	$5s^{2}5p^{6}4f5d 125027 2 (I-5)^{9}$	$5s^{2}5p^{6}4f6p^{2}25252.5(J-2)$	5.50E+09	0.33E+09	-0.14
895.002	58 5p +150 155027.2 (J=3) $5c^2 5p^6 4f5 d 131104 7 (J=3)^9$	$5s^{2}5n^{6}4f6n^{2}40077.0(J=4)$	0.97E+09	7.94E+09	-0.04
090.1 <i>31</i> 007.010	$5^{\circ}_{\circ}^{\circ$	$5s^{2}5n^{6}4f6n^{25}1562 O(I-2)$	1.80E+09	1.05E+09	-0.22
807.010	5s 5p 415d 140100.0 (J-2) $5c^2 5p^6 4f5d 125218 2 (J-2)^9$	$5s^{2}5n^{6}4f6n^{2}46677.6(J-4)$	1.60E+09	0.26E+09	-0.04
800 852	5s 5p 415d 155518.5 (J=5) $5s^2 5p^6 4f5d 127558 8 (J=2)^9$	$5s^{2}5n^{6}4f6n^{2}226880(1-2)$	9.02E+08	9.30E+08	-0.90
800.005	5s 5p 415d 127558.8 (J-2) $5s^2 5p^6 4f5d 127565 1 (J-4)^9$	5s 3p 410p 238088.0 (J=3) $5c^25n^64f6n 238688 0 (J=3)$	1.75E+09	1.07E+09	-0.07
000 549	$5_{0}^{2}5_{0}^{6}4f5d$ 125218 2 ($I=2$)	$5_{\rm s}^{2} 5_{\rm p}^{6} 4_{\rm f} 6_{\rm p} 246362.2 (J=3)$	1.00E+10	1.10E+10	0.10
000.040	$5_{\rm s}^{2}5_{\rm p}^{6}4f5d$ 135350 2 ($I=3$)	$5s^{2}5n^{6}4f6n^{2}46362.2(J=2)$	1.750 ± 09 $1.37E\pm00$	1.000 ± 0.00	-0.04
001 521	$5_{\rm s}^{2}5_{\rm p}^{6}4f5d$ 132162 1 (J=2) ²	$5s^{2}5p^{6}4f6p^{2}40502.2(J=2)$	1.3/E+09 1.87E+00	1.10E+09	-0.69
002 557	$5_{\rm s}^{2}5_{\rm p}^{6}Af^{2}$ 27/78 7 (1-2)	$5s^{2}5n^{6}Af5d$ 138275 A ($I=1$) ⁰	1.65E±09	2.77E+09	-0.12
902.337 004 700	$5_{0}^{2}5_{0}^{6}4f5d$ 122162 1 ($J=2$)	$5_{0}^{2} 5_{0}^{6} 4_{f} 6_{n} 2_{4}^{2} 2_{5}^{6} 4_{f} 6_{n} 2_{5}^{6} 4_{f} 2_{5}^{6} 4_{f} 6_{n} 2_{5}^{6} 4_{f} 2_{5}^$	1.0JE+08	2.24E+U8	-1.50
904./00	JS JP 41JU 152102.1 (J=4) [∞]	58 SP 410P 242094.9 (J=3)	J.7/E+09	1.23E+09	-0.08

5s²5p⁶4f6p 243087.0 (*J*=4)

5s²5p⁶4f6p 249919.6 (*J*=4)

5s²5p⁶4f6p 249730.1 (*J*=3)

5s²5p⁶4f6p 242694.9 (*J*=3)

5s²5p⁶4f6p 239232.5 (*J*=2)

5s²5p⁶4f6p 245187.5 (*J*=3)

5s²5p⁶4f6p 238688.0 (*J*=3)

9.38E+09 9.79E+09

1.87E+09 2.27E+09

6.37E+09 8.07E+09

4.93E+09

2.55E+09

4.97E+09

5.57E+08 1.16E+08 -1.87

6.10E+09

2.66E+09

6.08E+09

0.06

-0.57

-0.02

-0.15

-0.49

-0.15

 $5s^25p^64f5d \ 132597.5 \ (J=5)^o$

 $5s^25p^64f5d \ 139549.8 \ (J=3)^o$

5s²5p⁶4f5d 139549.8 (*J*=3)^o

5s²5p⁶4f5d 132565.8 (*J*=2)^o

5s²5p⁶4f5d 129104.5 (*J*=3)^o

5s²5p⁶4f5d 135318.3 (*J*=3)^o

5s²5p⁶4f5d 129104.5 (*J*=3)^o

905.068

906.045

907.601

908.034 908.034

910.176

912.542

$\lambda = (\mathring{A})^a$	Tran	aA ($\log(af)$		
Noos (11)	I ower level	Unner level	Previous ^a	HFR^{b}	HFR^{b}
912 837	$5s^25p^64f5d 140180 8 (I-2)^{\circ}$	$5s^25n^64f6n 249730 1 (I=3)$	4.78F+09	5.98F+09	-0.14
913 522	$5s^2 5p^6 4f^2 25892.9 (J=1)$	$5s^2 5p^6 4f5d 135359 2 (J=2)^{\circ}$	2 97E+08	3 57E+08	-1.28
917 947	$5s^2 5p^6 4f^2 26088 1 (J=6)$	$5s^2 5p^6 4f5d 135027.2 (J=5)^{\circ}$	6 30E+07	7 45E+07	-1.96
918 653	$5s^2 5p^6 4f5d 138275 4 (I=1)^{\circ}$	$5s^{2}5p^{6}4f6p 2471307 (J=1)$	1.93E+09	2 11F+09	-0.59
919 732	$5s^{2}5p^{6}4f5d 1343597 (J=4)^{o}$	$5s^{2}5p^{6}4f6p^{2}430870(J=4)$	2 85E+08	6 80F+08	-1.09
920 719	$5s^25p^64f5d 138519 2 (J=0)^{\circ}$	$5s^2 5p^6 4f6p 247130 7 (J=1)$	1.65E+09	1 93E+09	-0.63
921 212	$5s^2 5p^6 4f^2$ 20551 4 (<i>J</i> =2)	$5s^2 5p^6 4f5d 129104 5 (J=3)^{\circ}$	6.00E+06	9.09E+06	-2.86
923.053	$5s^25p^64f5d 134359.7 (J=4)^\circ$	$5s^25p^64f6p 242694.9 (J=3)$	9.30E+07	2.48E+08	-1.53
923.225	$5s^25p^64f^2$ 20050.6 (<i>J</i> =0)	$5s^25p^64f5d 133366.3 (J=1)^{\circ}$	1.41E+08	1.72E+08	-1.59
924.767	$5s^25p^64f5d 130553.0 (J=4)^\circ$	$5s^25p^64f6p 238688.0 (J=3)$	1.88E+09	2.69E+09	-0.49
924.844	$5s^25p^64f5d 131104.7 (J=3)^{\circ}$	$5s^25p^64f6p 239232.5$ (<i>J</i> =2)	1.90E+08	2.25E+08	-1.57
925.188	$5s^25p^64f5d \ 138275.4 \ (J=1)^o$	$5s^25p^64f6p 246362.2 (J=2)$	2.32E+09	2.93E+09	-0.44
925.415	$5s^25p^64f5d \ 135027.2 \ (J=5)^o$	$5s^25p^64f6p 243087.0 (J=4)$	2.81E+09	3.83E+09	-0.34
926.948	$5s^25p^64f^2$ 27478.7 (<i>J</i> =2)	$5s^25p^64f5d 135359.2 (J=2)^o$	2.40E+07	3.83E+07	-2.24
927.304	$5s^25p^64f^2$ 27478.7 (<i>J</i> =2)	$5s^25p^64f5d 135318.3 (J=3)^o$	1.55E+08	1.52E+08	-1.63
927.915	$5s^25p^64f5d 135318.3 (J=3)^{\circ}$	$5s^25p^64f6p 243087.0 (J=4)$	1.55E+09	2.06E+09	-0.60
930.460	$5s^25p^64f^2$ 25892.9 (<i>J</i> =1)	$5s^25p^64f5d 133366.3 (J=1)^o$	3.90E+07	5.62E+07	-2.07
931.296	$5s^25p^64f5d 135318.3 (J=3)^o$	$5s^25p^64f6p 242694.9 (J=3)$	2.90E+09	2.66E+09	-0.49
931.653	$5s^25p^64f5d \ 135359.2 \ (J=2)^o$	$5s^25p^64f6p 242694.9 (J=3)$	4.13E+09	4.79E+09	-0.23
934.508	$5s^25p^64f5d 142910.8 (J=5)^o$	$5s^25p^64f6p 249919.6 (J=4)$	1.19E+10	1.53E+10	0.28
934.508	$5s^25p^64f^2$ 20551.4 (<i>J</i> =2)	$5s^25p^64f5d$ 127558.8 (J=2)°	1.40E+08	1.22E+08	-1.73
936.233	$5s^25p^64f5d 139549.8 (J=3)^o$	$5s^25p^64f6p 246362.2 (J=2)$	7.70E+07	4.40E+07	-2.26
941.772	$5s^25p^64f5d 140180.8 (J=2)^o$	$5s^25p^64f6p 246362.2 (J=2)$	4.57E+08	4.62E+08	-1.22
944.586	$5s^25p^64f5d 133366.3 (J=1)^o$	$5s^25p^64f6p 239232.5 (J=2)$	2.59E+09	2.85E+09	-0.44
961.891	$5s^25p^64f5d 147601.4 (J=1)^o$	$5s^25p^64f6p 251563.0 (J=2)$	3.88E+09	4.95E+09	-0.18
963.694	$5s^25p^64f5d 142910.8 (J=5)^o$	$5s^25p^64f6p$ 246677.6 (<i>J</i> =4)	2.71E+09	3.01E+09	-0.39
975.470	$5s^25p^64f5d 140180.8 (J=2)^o$	5s ² 5p ⁶ 4f6p 242694.9 (<i>J</i> =3)	9.51E+08	7.96E+08	-0.96
998.232	5s ² 5p ⁶ 4f5d 142910.8 (<i>J</i> =5) ^o	5s ² 5p ⁶ 4f6p 243087.0 (<i>J</i> =4)	1.78E+09	3.01E+09	-0.39
1866.896	5s ² 5p ⁶ 4f6s 197997.9 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 251563.0 (<i>J</i> =2)	3.73E+09	4.17E+09	0.35
1868.031	5s ² 5p ⁶ 4f6s 193598.5 (<i>J</i> =2) ^o	5s ² 5p ⁶ 4f6p 247130.7 (<i>J</i> =1)	2.50E+09	2.47E+09	0.12
1895.243	5s ² 5p ⁶ 4f6s 193598.5 (<i>J</i> =2) ^o	5s ² 5p ⁶ 4f6p 246362.2 (<i>J</i> =2)	2.43E+09	2.15E+09	0.08
1899.414	5s ² 5p ⁶ 4f6s 194029.5 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 246677.6 (<i>J</i> =4)	4.76E+09	6.83E+09	0.58
1902.492	5s ² 5p ⁶ 4f6s 197452.8 (<i>J</i> =4) ^o	5s ² 5p ⁶ 4f6p 250015.7 (<i>J</i> =5)	6.24E+09	8.06E+09	0.65
1905.966	5s ² 5p ⁶ 4f6s 197452.8 (<i>J</i> =4) ^o	5s ² 5p ⁶ 4f6p 249919.6 (<i>J</i> =4)	1.88E+09	2.07E+09	0.07
1912.874	5s ² 5p ⁶ 4f6s 197452.8 (<i>J</i> =4) ^o	5s ² 5p ⁶ 4f6p 249730.1 (<i>J</i> =3)	1.57E+09	2.37E+09	0.13
1925.978	5s ² 5p ⁶ 4f6s 197997.9 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 249919.6 (<i>J</i> =4)	3.78E+09	4.51E+09	0.42
1933.032	5s ² 5p ⁶ 4f6s 197997.9 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 249730.1 (<i>J</i> =3)	2.71E+09	2.74E+09	0.20
1938.394	5s ² 5p ⁶ 4f6s 193598.5 (<i>J</i> =2) ^o	5s ² 5p ⁶ 4f6p 245187.5 (<i>J</i> =3)	2.79E+09	2.41E+08	-0.83
1954.726	5s ² 5p ⁶ 4f6s 194029.5 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 245187.5 (<i>J</i> =3)	1.55E+09	3.79E+08	-0.63
2030.842	5s ² 5p ⁶ 4f6s 197452.8 (<i>J</i> =4) ^o	5s ² 5p ⁶ 4f6p 246677.6 (<i>J</i> =4)	2.94E+08	3.37E+08	-0.66
2190.667	5s ² 5p ⁶ 4f6s 197452.8 (<i>J</i> =4) ^o	5s ² 5p ⁶ 4f6p 243097.0 (<i>J</i> =4)	1.86E+09	2.88E+09	0.32
2190.667	5s ² 5p ⁶ 4f6s 193598.5 (<i>J</i> =2) ^o	5s ² 5p ⁶ 4f6p 239232.5 (<i>J</i> =2)	1.02E+09	1.27E+09	-0.04
2209.637	5s ² 5p ⁶ 4f6s 197452.8 (<i>J</i> =4) ^o	5s ² 5p ⁶ 4f6p 242694.9 (<i>J</i> =3)	1.48E+09	1.63E+09	0.08
2211.551	5s ² 5p ⁶ 4f6s 194029.5 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 239232.5 (<i>J</i> =2)	1.08E+09	1.27E+09	-0.04
2217.127	5s ² 5p ⁶ 4f6s 193598.5 (<i>J</i> =2) ^o	5s ² 5p ⁶ 4f6p 238688.0 (<i>J</i> =3)	1.64E+09	1.47E+09	0.03
2217.127	5s ² 5p ⁶ 4f6s 197997.9 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 243087.0 (<i>J</i> =4)	1.63E+09	1.73E+08	-0.98
2236.596	5s ² 5p ⁶ 4f6s 197997.9 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 242694.9 (<i>J</i> =3)	1.16E+09	1.48E+09	0.05
2238.515	5s ² 5p ⁶ 4f6s 194029.5 (<i>J</i> =3) ^o	5s ² 5p ⁶ 4f6p 238688.0 (<i>J</i> =3)	1.25E+09	2.16E+09	0.20

Table D.1: Continued.

- ^a Meftah et al. (2008) and Delghiche et al. (2015)
- ^b Transition probabilities (gA) and oscillator strengths $(\log(gf))$ computed with HFR method (this work)

Appendix E

Comparison of the radiative parameters for Yb V

λ (Å) ^a	Lower 1	evel ^b		Upper le	evel ^b		Int ^c		$\log(qf)$)
	$E ({\rm cm}^{-1})$	P	J	$E (cm^{-1})$	P	J		Meftah ^d	HFR^{e}	MCDHF ^f
543.205	6112.03	(e)	4	190207.30	(0)	4	128	-0.98	-1.29	-1.51
543.205	9579.89	(0)	5	193671.10	(0)	6	128	-0.60	-0.72	-1.83
562.617	24192.89	(e)	4	201933.20	(0)	5	106	-0.41	-1.08	-0.68
564.458	6112.03	(e)	4	183275.10	(0)	5	146	-0.66	-1.23	-1.30
564.458	14405.00	(e)	4	191564.40	(0)	3	146	-0.99	-1.80	-1.10
567.252	0.00	(e)	6	176288.80	(0)	6	129	-0.58	-1.44	-1.50
567.743	9579.89	(e)	5	185715.70	(0)	5	102	-0.81	-0.94	-0.91
571.235	24192.89	(e)	4	199252.20	(0)	3	126	-0.55	-1.60	-0.71
571.235	43119.50	(e)	2	218177.80	(0)	1	126	-0.79	-1.75	-2.41
572.155	0.00	(e)	6	174778.00	(0)	6	116	-0.82	-1.09	-1.03
573.374	0.00	(e)	6	174405.80	(0)	5	109	-1.04	-1.29	-1.48
577.217	6112.03	(e)	4	179356.90	(0)	3	113	-0.85	-0.95	-1.04
578.449	6112.03	(e)	4	178991.40	(0)	5	138	-1.33	-1.97	-1.43
578.449	14405.00	(e)	4	187279.70	(0)	4	138	-0.96	-1.87	-2.13
580.547	0.00	(e)	6	172251.10	(0)	6	109	-0.91	-0.83	-1.06
581.140	9579.89	(e)	5	181655.20	(0)	5	112	-0.85	-1.29	-1.43
581.176	39037.90	(e)	6	211102.90	(0)	6	105	-0.62	-0.67	-0.29
583.541	6112.03	(e)	4	177478.10	(0)	3	107	-1.04	-1.38	-2.38
584.552	39037.90	(e)	6	210109.50	(0)	6	135	-0.01	-0.17	-0.80
589.608	6112.03	(e)	4	175716.10	(0)	3	107	-1.01	-1.28	-2.75
592.170	14405.00	(e)	4	183275.10	(0)	5	101	-0.88	-1.79	-1.42
594.713	9579.89	(e)	5	177728.40	(0)	5	113	-0.86	-0.67	-1.83
600.550	6112.03	(e)	4	172626.40	(0)	4	101	-1.10	-1.11	-1.29
802.074	161356.20	(0)	4	286033.82	(e)	5	167	-1.43	-1.64	-1.68
802.074	161356.20	(0)	4	286033.97	(e)	3	167	-1.90	-1.93	-1.35
864.742	143663.60	(0)	10	259305.05	(e)	9	171	0.68	0.65	0.61
868.304	153365.20	(0)	9	268532.23	(e)	8	158	0.63	0.61	0.56
870.582	145352.40	(0)	9	260218.14	(e)	8	156	0.47	0.45	0.40
872.274	159085.20	(0)	7	273728.28	(e)	6	115	0.12	0.26	0.20
873.216	164831.00	(0)	7	279350.06	(e)	6	117	0.42	0.40	0.26
873.996	154816.50	(0)	8	269233.49	(e)	7	136	0.40	0.37	0.32
877.540	146795.20	(0)	7	260750.18	(e)	7	105	0.08	-0.09	-0.09
877.557	145352.40	(0)	9	259305.05	(e)	9	134	0.11	0.09	0.04
877.868	164952.60	(0)	6	278864.67	(e)	5	116	0.01	-0.67	-1.30
878.807	155543.10	(0)	6	269333.95	(e)	6	101	0.10	0.11	0.01
879.385	154816.50	(0)	8	268532.23	(e)	8	113	0.11	0.09	0.04
879.385	146795.20	(0)	7	260509.01	(e)	6	113	-0.60	-0.79	-0.76
882.319	146880.70	(0)	8	260218.14	(e)	8	121	0.20	0.12	0.08
882.954	155977.30	(0)	7	269233.49	(e)	7	114	0.22	0.20	0.13
893.935	174169.40	(0)	3	286033.97	(e)	3	101	-0.68	-0.64	-0.76

7

5

6

7

6

7

7

(e)

(e)

(e)

(e)

(e)

(e)

(e)

101

107

103

162

160

160

132

-0.41

0.07

0.00

0.38

0.08

-0.16

-0.04

-0.30

0.08

0.07

0.36

0.10

-0.01

0.15

-0.41

0.05

0.02

0.35

-0.03

-0.11

0.06

893.935

895.390

896.212

898.672

904.534

904.534

905.246

145484.70

149901.50

145484.70

136614.90

149953.96

146795.20

146880.70

6

4

6

6

5

7

8

(0)

(0)

(0)

(0)

(0)

(0)

(0)

257348.77

261583.94

257065.63

247890.51

260509.01

257348.77

257348.77

Table E.1: Calculated oscillator strengths (log(gf)) for the strongest Yb V lines observed by Meftah et al. (2013)

$\frac{\lambda}{\lambda}$ (Å) ^a	Lowerl	evel ^b		Unner la	evel ^b		Int ^c		$\log(af)$)
<i>X</i> (11)	$E \text{ (cm}^{-1})$	P	J	$E (\mathrm{cm}^{-1})$	P	J	IIIt	$Meftah^d$	HFR^{e}	, MCDHF ^f
908 263	137790.20	(0)	7	247890 51	(e)	7	170	0.23	0.22	0.20
913.034	158053.00	(0)	6	267577.92	(e)	5	105	0.10	0.15	0.10
913 347	151021 29	(0)	6	260509.01	(e)	6	100	-0.08	-0.69	-0.80
917 234	152997 54	(0)	7	260000000000000000000000000000000000000	(e)	6	149	0.00	0.02	0.00
917 379	154789.62	(0)	6	262021.27	(e)	5	162	0.25	-0.02	-0.15
917.575	139582.60	(0)	9	248573.04	(e)	8	197	0.23	0.02	0.19
920 884	148757 30	(0)	8	257348 77	(e)	7	150	0.31	0.13	0.20
924 386	164006.60	(0)	7	272186 73	(e)	6	107	0.51	0.13	-0.11
925 770	154002 75	(0)	6	262021.27	(e)	6	107	-0.10	-0.49	-0.33
927 748	140784 80	(0)	8	248573.04	(c) (e)	8	102	0.10	0.42	0.33
932 508	150111 23	(0)	7	257348 77	(c) (e)	7	101	-0.11	-0.34	-0.25
933 656	140784.80	(0)	8	237340.77	(c) (e)	, 7	127	-0.11	-0.07	-0.23
935.050	160018 70	(0)	6	275541.01	(\mathbf{c})	5	127	-2.07	-0.02	-0.04
1/67 056	102628.22	(0)	8	273541.01	(\mathbf{c})	5 7	108	-2.07	-0.94	-0.81
1407.950	192028.22	(0)	0 7	262021.27	(\mathbf{c})	6	100	0.20	0.13	0.10
1470.889	194033.09	(0)	/ Q	260218.14	(\mathbf{c})	Q Q	200	0.07	-0.81	-0.50
1479.308	192028.22	(0)	0 5	200218.14	(e)	0 1	209	0.72	0.09	0.07
1404.200	208033.08	(0)	ך ר	270008.30	(e)	4	120	0.13	0.07	0.02
1403.030	202022.75	(0)	/ 5	209555.95	(e)	0	140	0.18	0.07	0.08
1407.033	212700.00	(0)	כ ד	279970.83	(e)	47	140	-0.04	-0.09	-0.01
1487.833	202022.75	(0)	1 5	209233.49	(e)	1	140	0.07	0.38	0.01
1487.902	200319.78	(0)	5 5	273728.28	(e)	0	119	0.55	0.21	0.16
1488.239	212/66.00	(0)	Э 4	279959.30	(e)	Э 4	152	0.06	0.11	-0.58
1489.834	212855.37	(0)	4	2/99/6.85	(e)	4	100	0.35	0.46	-0.32
1490.008	218920.29	(0)	4	286033.97	(e)	3	110	-0.05	-0.08	-0.13
1490.008	218920.29	(0)	4	286033.82	(e)	2	116	0.71	0.49	0.55
1490.233	212855.37	(0)	4	279959.30	(e)	2	134	-0.12	-0.8/	-0./1
1490.233	206519.78	(0)	5	273623.27	(e)	5	134	0.55	0.21	0.41
1492.096	208521.33	(0)	4	275541.01	(e)	5	125	0.30	-1.47	-1.14
1493.144	218920.29	(0)	4	285892.87	(e)	4	125	0.28	-0.36	-0.15
1494.048	206796.10	(0)	6	273728.28	(e)	6	132	0.57	0.52	0.48
1494.335	208635.08	(0)	5	275554.90	(e)	6	178	-3.22	-1.23	-1.58
1494.335	212855.37	(0)	4	279774.70	(e)	3	178	0.50	0.46	0.41
1494.629	208635.08	(0)	5	275541.01	(e)	5	115	0.45	0.34	0.11
1496.400	206796.10	(0)	6	273623.27	(e)	5	137	0.19	0.10	0.05
1496.875	202528.13	(0)	6	269333.95	(e)	6	169	0.67	0.62	0.55
1498.649	219307.35	(0)	3	286033.97	(e)	3	131	0.36	0.32	0.26
1498.909	194035.09	(0)	7	260750.18	(e)	7	193	0.74	0.68	0.66
1499.130	202528.13	(0)	6	269233.49	(e)	7	122	0.42	0.38	0.28
1499.774	192628.22	(0)	8	259305.05	(e)	9	283	0.97	0.94	0.91
1501.831	219307.35	(0)	3	285892.87	(e)	4	155	0.26	-0.20	-0.51
1501.859	212766.00	(0)	5	279350.06	(e)	6	189	0.78	0.76	0.27
1503.544	202022.73	(0)	7	268532.23	(e)	8	237	0.92	0.83	0.85
1504.282	206519.78	(0)	5	272996.60	(e)	4	179	0.59	0.46	0.46
1504.350	194035.09	(0)	7	260509.01	(e)	6	223	0.66	0.68	0.63
1505.571	206796.10	(0)	6	273216.25	(e)	7	218	0.86	0.80	0.79
1507.468	202528.13	(0)	6	268864.41	(e)	5	273	0.64	0.63	0.51
1510.967	194035.09	(0)	7	260218.14	(e)	8	282	0.50	0.46	0.41
1512.367	212855.37	(0)	4	278976.88	(e)	4	153	-0.08	0.03	0.30

0.26

0.39

-0.11

1512.894 212766.00 (o) 5 278864.67 (e) 5 166

Table E.1: Continued.

λ (Å) ^a	Lowerl	evel ^b		Unner le	evel ^b		Int ^c		$\log(af)$)
~ (23)	$E (\mathrm{cm}^{-1})$	P	J	$E (\mathrm{cm}^{-1})$	P	J	1110	Meftah ^d	HFR^e	
1514.937	212855.37	(0)	4	278864.67	(e)	5	136	0.11	0.26	0.19
1529.272	206796.10	(0)	6	272186.73	(e)	6	124	-0.50	-0.66	-0.28
1577.883	208635.08	(0)	5	272011.18	(e)	5	109	-0.93	-0.86	-2.03
1693.307	208521.33	(0)	4	267577.92	(e)	5	117	-0.96	-0.87	-0.78
1693.307	202528.13	(0)	6	261583.94	(e)	5	117	-0.55	-0.57	-0.51
1709.796	202022.73	(0)	7	260509.01	(e)	6	102	-0.64	-1.22	-0.37
1717.565	202528.13	(0)	6	260750.18	(e)	7	118	-0.83	-0.49	-0.75
1724.712	202528.13	(0)	6	260509.01	(e)	6	124	-0.62	-0.58	-0.68
1782.589	212766.00	(0)	5	268864.41	(e)	5	131	-0.84	-1.26	-1.27
1787.473	192628.22	(0)	8	248573.04	(e)	8	317	0.43	0.40	0.37
1801.748	206519.78	(0)	5	262021.27	(e)	6	393	0.41	0.38	0.37
1805.757	218920.29	(0)	4	274298.83	(e)	4	185	0.22	0.22	0.16
1807.469	202022.73	(0)	7	257348.77	(e)	7	295	0.33	0.21	0.24
1809.145	208521.33	(0)	4	263796.29	(e)	5	266	0.42	0.41	0.38
1809.556	192628.22	(0)	8	247890.51	(e)	7	500	0.69	0.67	0.64
1810.772	206796.10	(0)	6	262021.27	(e)	6	222	0.16	0.18	0.15
1812.862	208635.08	(0)	5	263796.29	(e)	5	235	0.24	0.23	-0.01
1816.071	206519.78	(0)	5	261583.94	(e)	5	789	0.05	-0.10	-0.10
1816.770	202022.73	(0)	7	257065.63	(e)	6	332	0.57	0.44	0.49
1817.108	212766.00	(0)	5	267798.48	(e)	4	254	0.40	-0.04	-0.10
1817.226	208521.33	(0)	4	263549.91	(e)	4	216	0.00	-0.02	-0.06
1818.464	219307.35	(0)	3	274298.83	(e)	4	271	0.20	0.18	0.10
1820.065	212855.37	(0)	4	267798.48	(e)	4	138	-0.01	0.40	-0.07
1821.004	208635.08	(0)	5	263549.91	(e)	4	217	0.38	0.38	0.16
1821.074	218920.29	(0)	4	273832.99	(e)	3	257	0.24	0.25	0.20
1824.134	202528.13	(0)	6	257348.77	(e)	7	321	0.56	0.50	0.44
1824.420	212766.00	(0)	5	267577.92	(e)	5	192	0.21	0.16	-0.25
1825.220	206796.10	(0)	6	261583.94	(e)	5	383	0.49	0.43	0.42
1827.394	212855.37	(0)	4	267577.92	(e)	5	221	0.34	0.27	0.20
1833.587	194035.09	(0)	7	248573.04	(e)	8	431	0.62	0.61	0.56
1833.587	202528.13	(0)	6	257065.63	(e)	6	431	0.04	-0.07	-0.12
1834.001	219307.35	(0)	3	273832.99	(e)	3	104	-0.18	-0.13	-0.17
1852.225	206519.78	(0)	5	260509.01	(e)	6	203	-0.24	-1.23	-0.90
1856.819	194035.09	(0)	7	247890.51	(e)	7	217	0.11	0.06	0.00
1861.745	206796.10	(0)	6	260509.01	(e)	6	103	-0.46	-1.06	-1.13

Table E.1: Continued.

- ^a Experimental wavelengths measured by Meftah et al. (2013).
- ^b Experimental levels as classified by Meftah et al. (2013) using their energy value, E, parity, P, and total quantum number, J.
- ^c Observed lines intensities (arbitrary units) as observed by Meftah et al. (2013). Only lines with Int > 100×10^6 s⁻¹ are listed in the table.
- ^d Oscillator strengths $(\log(gf))$ deduced from the transition probabilities (gA) calculated by Meftah et al. (2013).
- ^e $\log(gf)$ computed using the HFR method (this work)
- ^f $\log(gf)$ computed using the MCDHF method (this work)

Appendix F

Comparison of the radiative parameters for Lu V

	Lower lev	el^b		Upper leve	el^b		$gA(s^{-1})^{c}$		$\log gf^c$	
Wavelength $(Å)^a$	$E (cm^{-1})$	(P)	J	$E(cm^{-1})$	(P)	J	\mathbf{HFR}^{d}	MCDHF^{e}	HFR^d	MCDHF^{e}
504.825	0	(0)	7/2	198089	(e)	7/2	2.43E08*	1.80E08	-2.04*	-2.18
508.374	0	(0)	7/2	196706	(e)	5/2	2.96E08*	7.75E08	-1.95*	-1.54
511.664	0	(0)	7/2	195441	(e)	5/2	1.43E09	1.43E09	-1.26	-1.27
520.559	0	(0)	7/2	192100	(e)	9/2	5.63E07*	4.56E07#	-2.65*	-2.75#
523.569	0	(0)	7/2	190994	(e)	5/2	1.25E09	1.51E09	-1.30	-1.22
528.571	0	(0)	7/2	189188	(e)	7/2	8.00E07*	1.18E08#	-2.48*	-2.32#
535.277	0	(0)	7/2	186818	(e)	5/2	1.51E09	1.38E09	-1.19	-1.23
536.778	11793	(0)	5/2	198089	(e)	7/2	5.22E07*	4.53E07#	-2.65*	-2.72#
538.398	0	(0)	7/2	185736	(e)	7/2	3.99E07*	1.09E06#	-2.77*	-4.34#
540.794	11793	(0)	5/2	196706	(e)	5/2	1.19E08*	1.59E05#	-2.29*	-5.18#
544.518	0	(0)	7/2	183649	(e)	9/2	9.56E08	6.61E08#	-1.37	-1.53#
	11793	(0)	5/2	195441	(e)	5/2	1.91E09	1.54E09	-1.08	-1.18
549.375	0	(0)	7/2	182025	(e)	5/2	1.93E08*	2.08E07	-2.06*	-3.03
549 772	Ő	(0)	7/2	181894	(e)	7/2	5 14E08*	6 97E08	-1.63*	-1 50
555 444	ů 0	(0)	7/2	180036	(e)	7/2	2.69E09	4 00E09	-0.91	-0.73
558 024	0	(0)	7/2	179203	(e)	5/2	3 15E07*	2 58E09	-2 83*	-0.92
550.021	11793	(0)	5/2	100004	(e)	5/2	2 57E08*	1.12E08	_1.03*	-2.30
563 723	0	(0)	512 712	177306	(c) (e)	9/2	3 88F08	3 17E08#	-1.73	-2.50
505.725	0	(0)	217	177300	(\mathbf{c})	5/2	2.03E00	3 30E08	-1.75	-1.02π
	11703	(0)	5/2	180188	(\mathbf{c})	512 CIT	2.95E09 5.53E06*	1 30E07#	-0.80 2 58*	-1.00
560 200	0	(0)	512 7/2	175654	(\mathbf{c})	712 CLT	1.50E00	1.39207#	-3.36	-3.19π
571 246	11702	(0)	5/2	196919	(e)	5/2	1.39E09	1.93E09	-1.11	-1.03
571.540	11702	(0)	512	100010	(e)	512	1.00E09	0.40E09	-0.40	-0.51
574.902	11/95	(0)	512	185/30	(e)	712	1.19E08*	1.190E0/#	-2.23*	-2.42#
576.300	0	(0)	112	173520	(e)	112	2.17E09	1.18E09	-0.97	-1.23
580.580	0	(0)	9/2	172242	(e)	9/2	4.23E08	4.08E08	-1.6/	-1.68
583.746	0	(0)	112	1/130/	(e)	112	1.6/E09	1.22E09	-1.07	-1.21
584.778	0	(0)	7/2	171005	(e)	5/2	1.68E08*	3.81E08	-2.07*	-1.71
587.432	11793	(0)	5/2	182025	(e)	5/2	9.16E08	1.46E09	-1.33	-1.13
587.887	11793	(0)	5/2	181894	(e)	7/2	8.62E05*	9.55E06#	-4.35*	-3.30#
588.156	0	(0)	7/2	170023	(e)	5/2	5.66E08*	1.30E08	-1.53*	-2.17
594.380	11793	(0)	5/2	180036	(e)	7/2	2.04E09	1.68E09	-0.97	-1.05
597.338	11793	(0)	5/2	179203	(e)	5/2	7.72E08	3.85E07#	-1.38	-2.68#
598.004	0	(0)	7/2	167223	(e)	5/2	1.33E08*	5.25E06	-2.15*	-3.55
600.328	0	(0)	7/2	166577	(e)	5/2	1.63E08	2.56E08	-2.06	-1.86
600.470	0	(0)	7/2	166535	(e)	7/2	1.02E08*	1.18E08	-2.26*	-2.19
601.537	0	(0)	7/2	166240	(e)	9/2	1.44E09	9.59E08	-1.11	-1.28
609.013	0	(0)	7/2	164198	(e)	7/2	1.06E08*	1.69E05#	-2.23*	-5.02#
610.275	11793	(0)	5/2	175654	(e)	7/2	7.69E07*	1.58E08	-2.37*	-2.06
614.226	0	(0)	7/2	162806	(e)	9/2	2.12E09	1.47E09	-0.92	-1.07
615.162	0	(0)	7/2	162558	(e)	7/2	8.44E08	7.14E08	-1.32	-1.39
615.447	0	(0)	7/2	162483	(e)	9/2	1.40E08*	6.17E08	-2.10*	-1.45
617.384	0	(0)	7/2	161973	(e)	5/2	7.39E07*	8.93E07#	-2.37*	-2.29#
618.330	11793	(0)	5/2	173520	(e)	7/2	4.18E08*	3.99E08	-1.62*	-1.64
626.285	11793	(0)	5/2	171465	(e)	3/2	1.19E08*	1.12E08	-2.16*	-2.18
628.091	11793	(0)	5/2	171005	(e)	5/2	3.33E08	9.45E07	-1.71	-2.25
628.793	0	(0)	7/2	159035	(e)	7/2	7.29E08*	7.47E08	-1.37*	-1.35
628.998	0	(0)	7/2	158983	(e)	5/2	7.72E07	3.89E07#	-2.34	-2.62#
637.437	11793	(0)	5/2	168671	(e)	7/2	1.03E08*	1.63E08	-2.20*	-2.00
637.531	0	(0)	7/2	156855	(e)	9/2	4.46E08	1.57E08	-1.57	-2.02
640.120	0	(0)	7/2	156219	(e)	7/2	7.18E07*	1.41E07#	-2.36*	-3.06#
643.374	11793	(0)	5/2	167223	(e)	5/2	2.15E08*	6.96E07	-1.88*	-2.37
645.219	0	(0)	7/2	154985	(e)	9/2	2.86E08	4.81E08	-1.75	-1.51
646.060	11793	(0)	5/2	166577	(e)	5/2	1.01E08*	2.75E08	-2.20*	-1.76
646.238	11793	(0)	5/2	166535	(e)	7/2	1.03E08*	5.21E07#	-2.19*	-2.49#
647.581	0	(0)	7/2	154421	(e)	5/2	2.66E02*	1.64E06	-7.77*	-3.98
656.146	11793	(0)	5/2	164198	(e)	7/2	1.52E08	7.50E07	-2.01	-2.31
659.711	147970	(e)	15/2	299551	(0)	13/2	8.03E05*	8.85E05#	-4.29*	-4.30#
663.292	11793	(0)	5/2	162558	(e)	7/2	1.22E08*	2.18E08	-2.09*	-1.84

Table F.1: Transition probabilities (gA) and oscillator strengths $(\log gf)$ for experimentally observed lines in Lu V.

	Lower lev	el ^b		Unner lev	e^{1b}		$\sigma \Delta (s^{-1})^c$		log gf ^c	
Wavelength $(\mathring{A})^a$	$E (cm^{-1})$	(P)	Т	$E(cm^{-1})$	(P)	T	HER ^d	$MCDHF^{e}$	HFR^d	$MCDHF^{e}$
<u>664 182</u>		$\frac{(1)}{(0)}$	י כוד	150561	(I) (e)	י כוד	1 23E08*	1 34E08	_2 00*	-2.04
665 863	11703	(0)	5/2	161073	(\mathbf{c})	5/2	1.25E08 1.16E07*	1.54E08	-2.09	2.04
600.805	156663	(0)	15/2	200551	(\mathbf{c})	13/2	3.58E05*	3 53E05#	-5.11	-2.99
701 121	11702	(e)	5/2	154421	(0)	5/2	2.50E07*	3.33E03#	-4.50	-4.05#
701.121	11/95	(0)	3/2 12/2	134421	(e)	3/2	2.39E07* 7.26E04*	3.60E07	-2.12** 5.05*	-2.33
/11.801	139402	(e)	13/2	299879	(0)	0/2	7.30E04*	8.15E05#	-3.23*	-4.28#
/18.842	1/130/	(e)	112	310420	(0)	9/2	3.21E07	9.84E07	-2.60	-2.17
/5/.646	143/21	(e)	9/2	275709	(0)	9/2	1.44E08	4.13E08	-1.89	-1.50
786.582	160846	(e)	3/2	287980	(0)	5/2	7.85E07*	2.09E08	-2.13*	-1.77
790.958	143721	(e)	9/2	270150	(0)	11/2	1.16E09	1.64E09	-0.96	-0.86
791.571	154985	(e)	9/2	281316	(0)	11/2	3.38E08	8.23E08	-1.49	-1.15
793.168	143721	(e)	9/2	269797	(0)	9/2	1.02E08*	2.84E07#	-2.01*	-2.62#
798.330	162806	(e)	9/2	288068	(0)	9/2	6.79E08	7.94E08	-1.18	-1.17
798.984	162909	(e)	11/2	288068	(0)	9/2	5.63E08	8.03E08	-1.26	-1.16
803.460	156855	(e)	9/2	281316	(0)	11/2	1.22E09	9.96E08	-0.92	-1.05
804.510	157016	(e)	13/2	281316	(0)	11/2	5.71E08	7.00E08	-1.25	-1.21
804.715	143721	(e)	9/2	267988	(0)	11/2	1.12E09	3.63E08	-0.96	-1.50
805.483	151786	(e)	13/2	275935	(0)	11/2	8.48E08	1.09E09	-1.07	-1.02
806.043	160846	(e)	3/2	284908	(0)	5/2	5.67E08	1.06E09	-1.25	-1.03
807.412	150561	(e)	7/2	274413	(0)	5/2	5.23E08	3.44E08	-1.28	-1.53
808.779	162558	(e)	7/2	286201	(0)	9/2	1.94E08*	9.12E07	-1.71*	-2.09
811.908	154421	(e)	5/2	277587	(0)	5/2	3.29E07*	7.04E07	-2.49*	-2.21
813.433	161973	(e)	5/2	284908	(0)	5/2	4.34E08	5.82E08	-1.36	-1.28
814.355	157016	(e)	13/2	279813	(0)	13/2	9.82E08	9.72E08	-1.00	-1.05
817.741	147970	(e)	15/2	270258	(0)	13/2	2.36E09	2.18E09	-0.62	-0.70
818.952	166535	(e)	7/2	288642	(0)	7/2	3.86E08	3.40E08	-1.40	-1.51
819 642	164198	(e)	7/2	286201	(0)	9/2	2.64E08	6 54E08	-1.56	-1.23
820 249	159402	(e)	13/2	281316	(0)	11/2	2.06E09	1 78E09	-0.67	-0.79
821.643	148551	(e)	11/2	270258	(0)	13/2	5.15E09	5 44F09	-0.27	-0.30
821.750	163804	(e)	13/2	276256	(0)	11/2	7 95E08*	1 32E09	-1 09*	-0.91
822 378	148551	(e)	11/2	200400	(0)	11/2	1.47E08*	3.97E08	-1.82*	-1 44
822.578	154985	(c) (e)	9/2	276150	(0)	7/2	8 08E08*	4 11E08	-1.02	-1.43
822.497	166535	(C) (e)	212 CIT	270507	(0)	0/2	4.68E08	4.11E08	-2.00	-1.43
822.021	167125	(\mathbf{c})	0/2	288642	(0)	בוכ כוד	4.08E08	J.J8E08	-1.51	-1.29
822.930	167222	(e)	5/2	200042	(0)	712 CIT	2.04E08	4.40E08	-1.30	-1.40
825.393	167225	(e)	5/2	200042	(0)	712	4.34E08	J.19E08	-1.55	-1.55
825.428	100240	(e)	912 572	28/390	(0)	712	0.33E08	1.38E09	-1.18	-0.90
825.052	100005	(e)	512	280099	(0)	112 5 10	2.23E09	2.24E09	-0.03	-0.69
825.910	182025	(e)	5/2	303103	(0)	5/2	4./5E08	3.18E08	-1.31	-1.54
826.794	154985	(e)	9/2	275935	(0)	11/2	1.15E09	7.40E08	-0.92	-1.1/
827.260	155054	(e)	11/2	275935	(0)	11/2	2.49E09	1./3E09	-0.58	-0.79
827.442	166535	(e)	112	287390	(0)	7/2	5.19E08	5.02E08	-1.26	-1.33
828.845	165551	(e)	11/2	286201	(0)	9/2	5.45E08	8.28E08	-1.24	-1.11
829.830	176019	(e)	11/2	296526	(0)	11/2	1.51E09	1.36E09	-0.80	-0.89
830.408	147970	(e)	15/2	268393	(0)	15/2	2.51E09	1.96E09	-0.58	-0.74
830.492	159402	(e)	13/2	279813	(0)	13/2	8.43E08	4.48E08	-1.05	-1.37
831.499	167125	(e)	9/2	287390	(0)	7/2	1.36E09	7.20E08	-0.84	-1.17
832.149	154985	(e)	9/2	275157	(0)	7/2	1.24E09	5.01E08	-0.89	-1.33
833.538	168671	(e)	7/2	288642	(0)	7/2	7.69E08	3.35E08	-1.09	-1.51
833.931	177396	(e)	9/2	297310	(0)	9/2	6.54E08	7.71E08	-1.15	-1.13
834.694	143721	(e)	9/2	263525	(0)	9/2	5.08E08	5.92E08	-1.27	-1.27
836.108	143721	(e)	9/2	263323	(0)	7/2	2.52E08	2.59E08	-1.58	-1.63
836.289	168491	(e)	11/2	288068	(0)	9/2	2.61E09	2.67E09	-0.55	-0.60
837.382	166535	(e)	7/2	285954	(0)	7/2	2.40E06*	1.05E09	-3.58*	-0.99
838.674	150561	(e)	7/2	269797	(0)	9/2	2.13E06*	8.43E08	-3.63*	-1.10
839.780	156855	(e)	9/2	275935	(0)	11/2	3.31E08	6.59E08	-1.44	-1.20
840.916	157016	(e)	13/2	275935	(0)	11/2	3.60E09	3.29E09	-0.41	-0.51
841.366	156855	(e)	9/2	275709	(o)	9/2	2.61E08*	6.26E08	-1.55*	-1.22

841.544

843.058

167125

168671

9/2

7/2

(e)

(e)

285954

287287

7/2

5/2

(0)

(0)

2.25E07*

5.50E08

1.24E09

1.80E08

-0.92

-1.76

-2.61*

-1.22

1	90	
_	/ 0	

	Lower leve	el^b		Upper leve	el^b		$gA(s^{-1})^{c}$		$\log \mathfrak{g} \mathfrak{f}^c$	
Wavelength $(\text{\AA})^a$	$E(cm^{-1})$	(P)	J	$E(cm^{-1})$	(P)	J	HFR^{d}	MCDHF^{e}	HFR^{d}	MCDHF^{e}
843.503	159035	(e)	7/2	277587	(0)	5/2	7.23E07*	1.65E08	-3.08*	-1.81
843.810	162806	(e)	9/2	281316	(0)	11/2	1.05E09	6.92E08	-0.94	-1.17
844.079	151786	(e)	13/2	270258	(0)	13/2	1.89E09	2.13E09	-0.69	-0.68
844.543	162909	(e)	11/2	281316	(0)	11/2	1.05E09	1.37E09	-0.94	-0.87
844.852	151786	(e)	13/2	270150	(0)	11/2	4.06E08*	9.00E08	-1.35*	-1.06
845.296	156855	(e)	9/2	275157	(0)	7/2	2.09E06*	1.27E07#	-3.64*	-2.91#
846.067	156219	(e)	7/2	274413	(0)	5/2	4.55E08	3.72E08	-1.31	-1.45
847.460	162806	(e)	9/2	280805	(0)	9/2	2.83E08*	5.63E08	-1.50*	-1.26
848.206	162909	(e)	11/2	280805	(0)	9/2	1.81E09	1.35E09	-0.70	-0.87
848.824	158125	(e)	11/2	275935	(0)	11/2	1.16E09	1.49E09	-0.89	-0.84
849.545	168491	(e)	11/2	286201	(0)	9/2	7.14E08	8.26E08	-1.10	-1.09
849.723	167223	(e)	5/2	284908	(0)	5/2	1.17E09	2.85E08	-0.89	-1.55
850.057	193214	(e)	17/2	310853	(0)	15/2	3.38E10	3.52E10	0.57	0.53
850.458	158983	(e)	5/2	276567	(0)	7/2	2.20E08	4.31E07	-1.62	-2.39
	158125	(e)	11/2	275709	(0)	9/2	7.59E08	4.04E08	-1.08	-1.40
850.836	159035	(e)	7/2	276567	(0)	7/2	7.50E06*	5.68E08	-3.08*	-1.26
850 976	163804	(e)	13/2	281316	(0)	11/2	2 77E08	5 47E08	-1 51	-1.26
851 580	170639	(e)	9/2	288068	(0)	9/2	3 55E09	4 09E09	-0.40	-0.39
852 001	150561	(e)	7/2	260000	(0)	9/2	5 39E09	5.64E09	-0.23	-0.26
002.001	185736	(e)	7/2	303103	(0)	5/2	6 13E08	1 77E09	-1.17	-0.76
852 267	171307	(e)	7/2	288642	(0)	7/2	1 11E09	9.69E08	-0.91	-1.03
852.207	180036	(e)	7/2	200012	(0)	9/2	1.41E09	1.25E09	-0.80	-0.90
853 379	156219	(e)	7/2	273400	(0)	9/2	5 94F08	3.87E08	-1 19	-1 42
855 408	162909	(c) (e)	11/2	279813	(0)	13/2	1 15E09	9 32F08#	-0.89	-1.02#
856 592	160846	(c) (e)	3/2	277587	(0)	5/2	3 15E09	3.61F08	-1.46	-1.46
857 582	151786	(c) (e)	13/2	268393	(0)	15/2	1 71E00	1 31F09#	-0.71	-0.88#
057.502	164198	(c) (e)	7/2	280805	(0)	9/2	3.05E09	2 07F09	-0.46	-0.69
858 039	156855	(c) (e)	9/2	273400	(0)	9/2	7 71F08	6.13E08	-1.07	-1.21
858 128	159402	(e)	13/2	275935	(0)	11/2	1.07E09	1 18F09	-0.92	-0.93
859 109	172242	(c) (e)	9/2	273733	(0)	7/2	1.07E07	2 11F09	-0.92	-0.99
859.109	158083	(c) (e)	5/2	200042	(0)	5/2	1.00E09	1 21E09	-0.07	-0.02
860 567	151786	(c) (e)	13/2	275205	(0)	11/2	2 35E09	1.21E09	-0.50	-0.75
860 781	158083	(c) (e)	5/2	207200	(0)	7/2	2.55E07 2.11E09	2 15E09	-0.50	-0.70
861 164	150035	(C) (e)	512 712	275157	(0)	712	2.11E09 2.01E09	2.13E09 1.07E09	-0.62	-0.08
861.455	171307	(c)	712 CIT	273137	(0)	712	2.01E09 0 56E08	1.07E09	-0.04	-0.97
861.024	152272	(e)	17/2	267390	(0)	15/2	9.50E08	1.80E09	-0.90	-0.73
862 222	171207	(e)	1/12 7/2	200393	(0)	5/2	3.27E10 3.52E00	4 33E00	0.37	0.33
862.222	16/108	(e)	712 CIT	287287	(0)	512 CIT	1.26E09	4.33E09	-0.40	-0.30
862 270	104190	(e)	0/2	200099	(0)	0/2	1.20E09	1.47E09	-0.64	-0.85
866 324	172242	(e)	5/2	200000	(0)	5/2	2.30E08	1.80E08	-1.30	-1.74
866 028	150905	(e)	15/2	274413	(0)	12/2	1.29E09	2.86E08	-0.85	-1.24
800.928	159125	(e)	13/2	279015	(0)	0/2	2.03E10 1.22E08*	2.89E10	1.96*	1.02
007.407 868.022	155054	(e)	11/2	273400	(0)	912 12/2	1.22E08 ¹	9.24E08	-1.80*	-1.03
000.025 969 227	153034	(e)	0/2	270238	(0)	15/2	1.40E09	1.40E09	-0.79	-0.84
000.321	134983	(e)	9/2	270130	(0)	11/2	7.81E08	2.50E09	-1.03	-0.05
000.447	172520	(e)	912 CIE	201390	(0)	712 CLT	2.02E09	1.95E09	-0.05	-0.70
000.032	173920	(e)	112 510	200042	(0)	112 5 /0	1.1/E09	2.13E09	-0.87	-0.00
868.841	1/2885	(e)	5/2	28/980	(0)	5/2	1.04E09	6.06E07	-0.92	-2.21
969 002	155054	(e)	0/2	2/0150	(0)	11/2	2.00E09	4.91E09	-0.64	-0.30
868.993	166240	(e)	9/2	281310	(0)	11/2 5/2	1.82E09	2.19E09	-0.67	-0.65
809.347	102338	(e)	11/2	211381	(0)	5/2	3./3E08	1.37E08	-1.57	-1.8/
869.760	148551	(e)	11/2 5/0	263525	(0)	9/2	1.11E09	1.03E09	-0.90	-0.99
809.949	170022	(e)	512	283934	(0)	112	0.09EU8	2.07E09	-0.99	-0.0/
870.436	170023	(e)	5/2	284908	(0)	5/2	3.43E08	3.18E09	-1.40	-0.48
870.836	189188	(e)	7/2	304021	(0)	1/2	7.51E08	2.86E08	-1.06	-1.53
870.990	154985	(e)	9/2	269797	(0)	9/2	5.30E00*	5.26E08	-9.21*	-1.27
070 101	181894	(e)	7/2	296706	(0)	7/2	7.02E09	6.94E09	-0.08	-0.14
872.194	161055	(e)	11/2	275709	(0)	9/2	3.39E09	6.90E09	-0.40	-0.15
872.647	161973	(e)	5/2	276567	(0)	7/2	2.62E08	1.26E09	-1.52	-0.89
872.869	166240	(e)	9/2	280805	(0)	9/2	3.15E09	5.83E09	-0.43	-0.22
873.323	172885	(e)	5/2	287390	(0)	7/2	1.25E09	1.38E09	-0.83	-0.85
873.840	158983	(e)	5/2	273421	(0)	7/2	2.76E09	3.92E09	-0.50	-0.40

	Lower leve	el ^b		Unner leve	1 ^b		$\sigma A (s^{-1})^c$		log of ^c	
Wavelength $(\text{\AA})^a$	$E (cm^{-1})$	(P)	Т	$E(cm^{-1})$	(P)	T	HFR^d	$MCDHF^{e}$	HFR^d	$MCDHF^{e}$
874 237	159035	(r) (e)	י כוד	273421	$\frac{(1)}{(0)}$	3 7/2	7 85E08	7 96F08	-1.05	-1.09
874 319	198972	(c) (e)	9/2	313347	(0)	11/2	7.05E00	6.97E09	-0.08	-0.15
874 638	181894	(e)	7/2	296226	(0)	5/2	1.45E09	1 84F09	-0.77	-1 72
875 121	166535	(e)	7/2	290220	(0)	9/2	1.43E09	6.93E08	-0.84	-1.13
875.645	182025	(\mathbf{c})	5/2	200005	(0)	5/2	1.21E09	0.95E08	0.28	-1.13
875 724	167125	(c) (e)	9/2	290220	(0)	11/2	1.00E09	1.36E09	-0.20	-1.85
875 892	182357	(c) (e)	13/2	201510	(0)	11/2	2.41E10	2.42E10	0.45	0.40
876 449	174544	(c) (e)	9/2	290520	(0)	7/2	4 57E08*	2.42E10 2.59E08	_1 27*	-1 58
876 548	162483	(e)	9/2	276567	(0)	7/2	3.61E08	2.37E00 4 24E09	-1.38	-0.36
877 127	162558	(e)	7/2	276567	(0)	7/2	5 78E07*	2.63E08	-2 17*	-1 57
877 501	172242	(e)	9/2	286201	(0)	9/2	3 39F09	2.05E00 4.81E09	-0.40	-0.30
877 848	189188	(e)	7/2	303103	(0)	5/2	9.81E09	8 98F09	0.40	-0.03
877 933	171005	(e)	5/2	284908	(0)	5/2	3 48E09	1 34E09	-0.38	-0.85
878 199	173520	(e)	7/2	287390	(0)	7/2	9.46E08	6 49E08	-0.95	-1.17
878 279	166240	(e)	9/2	280099	(0)	7/2	1 86E08*	4 60E08	-1 66*	-1.32
879 409	172242	(e)	9/2	285954	(0)	7/2	1.80E00	5 85E09	-2.65*	-0.21
879.666	167125	(e)	9/2	280805	(0)	9/2	3 26E09	1 10E09	-0.41	-0.93
880 316	156663	(e)	15/2	270258	(0)	13/2	1 80E10	1 77E10	0.33	0.27
880.457	156219	(e)	7/2	269797	(0)	9/2	1.61E08	1.08E08	-1.72	-1.94
880.543	166535	(e)	7/2	280099	(0)	7/2	5.51E09	4.98E09	-0.18	-0.27
	160846	(e)	3/2	274413	(0)	5/2	4.44E09	3.84E09	-0.28	-0.40
880.610	161973	(e)	5/2	275530	(0)	3/2	7.55E08	7.48E08	-1.06	-1.12
880.873	174544	(e)	9/2	288068	(0)	9/2	2.73E09	2.10E09	-0.49	-0.66
881.434	162483	(e)	9/2	275935	(0)	11/2	7.92E08	6.92E08	-1.02	-1.14
881.497	171465	(e)	3/2	284908	(0)	5/2	3.81E09	3.57E09	-0.34	-0.42
882.537	161973	(e)	5/2	275283	(0)	5/2	5.39E08	4.41E08	-1.20	-1.34
882.654	156855	(e)	9/2	270150	(0)	11/2	3.90E08	4.61E08	-1.33	-1.31
882.963	172242	(e)	9/2	285495	(0)	11/2	5.55E08	5.07E08	-1.17	-1.27
883.065	157016	(e)	13/2	270258	(0)	13/2	6.32E09	6.04E09	-0.12	-0.20
883.520	161973	(e)	5/2	275157	(0)	7/2	2.44E09	1.69E09	-0.54	-0.75
883.609	174895	(e)	7/2	288068	(0)	9/2	2.78E08	2.64E08	-1.48	-1.55
883.914	157016	(e)	13/2	270150	(0)	11/2	1.98E07*	1.18E09	-2.62*	-0.91
884.111	164479	(e)	3/2	277587	(0)	5/2	9.11E07	3.62E08	-1.96	-1.43
884.207	184215	(e)	11/2	297310	(0)	9/2	1.36E10	1.37E10	0.22	0.16
884.290	174895	(e)	7/2	287980	(0)	5/2	1.08E09	1.91E09	-0.88	-0.70
	171307	(e)	7/2	284393	(0)	9/2	5.01E07*	5.51E07	-2.23*	-2.23
884.512	183649	(e)	9/2	296706	(0)	7/2	6.39E09	6.35E09	-0.11	-0.17
884.747	190994	(e)	5/2	304021	(0)	7/2	1.91E08	1.92E08	-1.64	-1.70
884.928	154985	(e)	9/2	267988	(0)	11/2	1.51E09	1.22E09	-0.75	-0.89
885.057	175654	(e)	7/2	288642	(0)	7/2	1.11E09	7.33E08	-0.88	-1.11
885.160	167125	(e)	9/2	280099	(0)	7/2	2.43E08*	5.04E07#	-1.53*	-2.27#
885.235	150561	(e)	7/2	263525	(0)	9/2	2.96E09	3.67E09	-0.46	-0.42
885.394	156855	(e)	9/2	269797	(0)	9/2	4.56E07*	1.29E09	-2.26*	-0.86
885.720	162806	(e)	9/2	275709	(0)	9/2	4.85E07*	4.49E08	-2.23*	-1.33
885.923	183649	(e)	9/2	296526	(0)	11/2	9.45E08	7.70E08#	-0.94	-1.08#
886.160	143721	(e)	9/2	256566	(0)	11/2	1.41E10	1.58E10	0.22	0.21
	174544	(e)	9/2	287390	(0)	7/2	9.68E09	9.37E09	0.07	0.00
886.322	168491	(e)	11/2	281316	(0)	11/2	8.07E09	7.82E09	-0.01	-0.08
886.438	168506	(e)	13/2	281316	(0)	11/2	1.47E10	1.42E10	0.25	0.18
886.533	162909	(e)	11/2	275709	(0)	9/2	1.03E09	1.53E09	-0.90	-0.79
886.824	150561	(e)	7/2	263323	(0)	7/2	3.79E09	3.33E09	-0.35	-0.47
887.517	162483	(e)	9/2	275157	(0)	7/2	7.37E09	2.95E09	-0.05	-0.51
888.110	162558	(e)	7/2	275157	(0)	7/2	5.19E09	5.54E09	-0.21	-0.23
888.932	174895	(e)	7/2	287390	(0)	7/2	1.92E09	1.85E09	-0.63	-0.70
889.359	161973	(e)	5/2	274413	(0)	5/2	1.98E09	2.18E09	-0.62	-0.64
889.410	1/3520	(e)	1/2	285954	(0)	1/2	1.89E04*	1.57E09	-5.64*	-0.77
889.923	164198	(e)	1/2	276567	(0)	1/2	1.92E09	1.74E09	-0.64	-0.74
890.068	162806	(e)	9/2	2/5157	(0)	1/2	2.22E08	5.13E09	-1.57	-0.48
890.114	101055	(e)	11/2	2/3400	(0)	9/2	1.00E10	0.44E09	0.08	-0.16
890.360	168491	(e)	11/2	280805	(0)	9/2	8.28E09	8.48E09	0.01	-0.04

191

	Lower lev	el ^b		Unner leve	1 ^b		$\sigma A (s^{-1})^c$		log of ^c	
Wavelength $(\text{\AA})^a$	$E(cm^{-1})$	(P)	T	$E (cm^{-1})$	(P)	T	HFR^d	$MCDHF^{e}$	HFR^d	$MCDHF^{e}$
891 814	163804	(r) (e)	13/2	275935	(1)	11/2	1.81F10	1 77F10	$\frac{111}{0.34}$	0.28
801 001	100004	(c) (e)	5/2	303103	(0)	5/2	3 21E00	3 14E09	-0.41	-0.47
892 556	201310	(c) (e)	11/2	313347	(0)	11/2	3.44E08	6 52E09	-1.38	-0.47
892.556	158125	(c) (e)	11/2	270150	(0)	11/2	2.18E00	3 23E00	0.57	-0.15
692.050	197526	(\mathbf{c})	15/2	200551	(0)	13/2	2.10E09	2.71E10	-0.57	-0.40
803 480	107520	(e)	0/2	299551	(0)	13/2	2.39E10	2.71E10 1.61E10	0.45	0.43
804 013	162558	(e)	212 CIT	274412	(0)	5/2	2.34E00	2 10E00	0.50	0.24
894.013	102338	(e)	15/2	274413	(0)	15/2	2.34E09	2.10E09	-0.54	-0.03
895.014	156210	(e)	13/2	200393	(0)	0/2	9.30E09	9.40E09	0.00	0.02
095.152 805.470	150219	(e)	11/2	201952	(0)	912	0.94E09	0.23E09	-0.08	-0.17
895.470	136123	(e)	5/2	209797	(0)	912 CLF	4.04E08	2.31E09	-1.51	-0.00
891.282	101973	(e)	312	273421	(0)	0/2	2.80E09	2.70E09	-0.47	-0.34
907 400	198972	(e)	912 7/2	280000	(0)	912 CLF	9.00E09	9.79E09	0.08	0.03
897.422	1080/1	(e)	7/2	280099	(0)	112 5 10	2.55E08	5.16E08	-1.50	-1.24
897.766	173520	(e)	112	284908	(0)	5/2	1.26E09	1.46E09	-0.81	-0.79
897.857	15/016	(e)	13/2	268393	(0)	15/2	5.63E08	4.44E08#	-1.10	-1.31#
898.301	168491	(e)	11/2	279813	(0)	13/2	7.09E08	5.11E08#	-1.05	-1.25#
898.415	168506	(e)	13/2	279813	(0)	13/2	8.10E09	7.96E09	0.01	-0.05
898.918	17/396	(e)	9/2	288642	(0)	7/2	4.54E09	2.54E09	-0.25	-0.57
898.980	176831	(e)	11/2	288068	(0)	9/2	1.59E10	1.58E10	0.30	0.24
899.489	202173	(e)	11/2	313347	(0)	11/2	1.25E10	7.02E09	-0.71	-0.11
899.817	156855	(e)	9/2	267988	(0)	11/2	2.42E09	9.66E08	-0.53	-0.97
900.213	164198	(e)	7/2	275283	(0)	5/2	1.64E09	9.93E08	-0.70	-0.98
900.271	156855	(e)	9/2	267932	(0)	9/2	7.55E09	4.84E09	-0.03	-0.27
900.812	166577	(e)	5/2	277587	(0)	5/2	9.59E08	1.71E08	-0.93	-1.74
901.126	157016	(e)	13/2	267988	(0)	11/2	1.22E10	1.25E10	0.17	0.13
901.232	164198	(e)	7/2	275157	(0)	7/2	6.54E06*	7.98E05#	-3.09*	-4.07#
901.582	162483	(e)	9/2	273400	(0)	9/2	3.62E09	1.33E09	-0.36	-0.84
902.185	162558	(e)	7/2	273400	(0)	9/2	1.37E09	5.60E08	-0.78	-1.22
902.499	164479	(e)	3/2	275283	(0)	5/2	2.98E09	2.90E09	-0.44	-0.51
902.833	203211	(e)	15/2	313974	(0)	13/2	1.60E10	1.56E10	0.30	0.24
902.954	159402	(e)	13/2	270150	(0)	11/2	1.48E10	1.10E10	0.27	0.08
904.594	175654	(e)	7/2	286201	(0)	9/2	3.44E08	6.51E08	-1.36	-1.13
905.047	162909	(e)	11/2	273400	(0)	9/2	5.55E08	4.20E08	-1.16	-1.33
906.082	167223	(e)	5/2	277587	(0)	5/2	6.45E08	1.55E09	-1.09	-0.77
906.619	175654	(e)	7/2	285954	(0)	7/2	2.54E08*	1.63E09	-1.49*	-0.73
907.554	203161	(e)	13/2	313347	(0)	11/2	9.02E09	8.47E09	0.06	-0.02
907.718	170639	(e)	9/2	280805	(o)	9/2	2.30E09	1.40E09	-0.53	-0.79
908.460	170023	(e)	5/2	280099	(o)	7/2	1.06E09	7.55E08	-0.87	-1.07
908.988	178629	(e)	9/2	288642	(0)	7/2	8.44E09	1.02E10	0.03	0.06
909.637	164479	(e)	3/2	274413	(0)	5/2	7.91E08	1.16E09	-1.00	-0.89
909 941	177390	(e)	5/2	287287	(0)	5/2	4 22E08	8 32E07	-1 27	-2.03
910 156	181894	(e)	7/2	291764	(0)	5/2	1 89E09	3 05E09	-0.64	-0.49
910 220	158125	(e)	11/2	267988	(0)	11/2	6 20E09	3 15E09	-0.11	-0.45
910.683	158125	(e)	11/2	267932	(0)	9/2	4 78E09	3 48E09	-0.22	-0.41
911 242	182025	(e)	5/2	201764	(0)	5/2	5.07E08	1.09F08#	-1.20	-1 92#
911.2.12	182025	(e)	5/2	291733	(0)	3/2	1.69E09	1 34F09	-0.68	-0.83
012 834	102023	(c) (e)	5/2	30/000	(0)	5/2	2 27E00	2 73E00	0.55	0.52
013 560	170630	(C) (A)	9/2	280000	(0)	בוב כוד	4 32E00	2.75E07	0.25	-0.32
013 720	167125	(\mathbf{c})	0/2	280099	(0)	217	4.32E09	4.30E09	-0.25	-0.50
014 012	186818	(\mathbf{c})	5/2	270307	(0)	5/2	4.30E09	1.04E09	-0.20	-0.09
01/ 376	176821	(c) (a)	11/2	220220	(0)	012	2.72E00 8 56E09	5.22E00 5.34E09	-1.45	-1. 4 5 _1.71
014.520	1/0001	(C) (a)	15/2	200201	(0)	<i>コレ</i> 12/2	0.JULU0 2 21E10	2.24EU0 2.44E10	-0.95	-1.21
015 720	14/2/0	(C) (a)	1312 017	231293 272100	(0)	0/2	2.21110 5 04E00	2.77E10 1.04E00	1 20	0.43
915.750	104190		11/2	273400	(0)	712 12/2	2.04EU0 8.65E07	1.04E09	-1.20	-0.94 2.06#
016 502	201210	(e)	11/2	210238	(0)	13/2	0.0JEU/ 1.21E00*	1.02EU/#	-1.93 1 77*	-2.00#
910.303	201310	(e)	11/2	310420 375520	(0)	912 212	1.51EU8*	1./JEU9	-1.//*	-0.09
917.821	1003//	(e)	312 0/2	2/3330	(0)	312 7/2	1.12E09	0.31EU0#	-0.85	-5.14#
918.131	100240	(e)	912 510	2/313/	(0)	112	2.34EU0*	3.19EU8	-3.52*	-1.45
918.260	154421	(e)	5/2	203323	(0)	112	7.01E09	/.1/E09	-0.05	-0.10
919.0/1	1//396	(e)	9/2	286201	(0)	9/2	3.62E08	1.40E08	-1.33	-1.79

	Lower law	a^{1b}		Upper law	1 ^b		$\alpha \Lambda (c^{-1})c$		log gfc	
Wavelength $(\mathring{A})^{q}$	$E (am^{-1})$		т	$E (am^{-1})$	(D)	т	$g_{A}(s)$	MCDUE		MCDHE
wavelength (A)*	$E(\text{cm}^{-1})$	(P)	J	E (cm)	(P)	J		MCDHF [®]	HFK ²	MCDHF*
919.557	166535	(e)	112	275283	(0)	5/2	2.33E09	3.09E09	-0.53	-0.46
919.607	148551	(e)	11/2	257293	(0)	13/2	3.36E09	3.25E09	-0.37	-0.44
919.909	166577	(e)	5/2	275283	(0)	5/2	2.33E09	9.97E08	-0.53	-0.95
920.269	176831	(e)	11/2	285495	(0)	11/2	7.09E08	7.06E08	-1.03	-1.08
920.621	166535	(e)	7/2	275157	(0)	7/2	1.70E08	3.73E08	-1.65	-1.37
920.925	159402	(e)	13/2	267988	(0)	11/2	1.68E09	5.87E09	-0.67	-0.17
921.116	172242	(e)	9/2	280805	(0)	9/2	3.85E08	4.09E08	-1.30	-1.32
921.319	154985	(e)	9/2	263525	(0)	9/2	6.60E09	6.09E09	-0.08	-0.17
921.898	155054	(e)	11/2	263525	(0)	9/2	1.15E10	1.07E10	0.17	0.08
922.727	176019	(e)	11/2	284393	(0)	9/2	5.51E09	1.06E10	-0.15	0.08
923.042	154985	(e)	9/2	263323	(0)	7/2	3.50E09	2.45E09	-0.35	-0.56
923.492	196706	(e)	5/2	304990	(0)	5/2	5.80E08	1.87E08	-1.13	-1.67
923.812	202173	(e)	11/2	310420	(0)	9/2	3.73E09	1.79E09	-0.31	-0.68
925.408	167223	(e)	5/2	275283	(0)	5/2	2.52E08	1.83E09	-1.49	-0.68
925.655	167125	(e)	9/2	275157	(0)	7/2	1.75E08*	1.46E09	-1.64*	-0.78
925.787	148551	(e)	11/2	256566	(0)	11/2	9.95E09	1.10E10	0.11	0.10
926 489	167223	(e)	5/2	275157	(0)	7/2	1 49E08	8 72E08	-171	-0.99
926.815	168671	(e)	7/2	276567	(0)	7/2	1 37E08	3 45E08	-1 74	-1 40
926.019	177396	(e)	9/2	285271	(0)	7/2	4.06E06*	4 26F09	-3.27*	-0.30
920.999	165551	(e)	11/2	273400	(0)	9/2	4 30F00	9.01F09	-0.24	0.00
929.005	203211	(c) (e)	15/2	310853	(0)	15/2	9.66E00	0.64E00#	0.11	0.02
929.005	178620	(\mathbf{c})	0/2	286201	(0)	0/2	3.61E00	2 53E00	0.11	0.00#
929.000	170023	(e)	5/2	280201	(0)	5/2	1.08E00	2.33E09	-0.52	-0.32
929.070	170025	(e)	512	277387	(0)	3/2	1.98E09	3.00E08	-0.38	-1.24
931.384	162800	(e)	912	270150	(0)	11/2	2.81E09	2.14E09	-0.43	-0.60
931.917	156219	(e)	112	263525	(0)	9/2	4.16E08	5.04E08	-1.27	-1.24
932.915	16/223	(e)	5/2	274413	(0)	5/2	4.10E08	1.01E08	-1.26	-1.93
933.007	166240	(e)	9/2	273421	(0)	7/2	2.97E09	1.55E09	-0.41	-0.74
933.182	166240	(e)	9/2	273400	(0)	9/2	2.15E09	1.43E09	-0.55	-0.78
933.672	156219	(e)	7/2	263323	(0)	7/2	3.57E09	4.48E09	-0.33	-0.29
934.647	162806	(e)	9/2	269797	(0)	9/2	6.69E09	4.95E09	-0.05	-0.23
935.448	198089	(e)	7/2	304990	(0)	5/2	5.38E09	4.42E09	-0.15	-0.30
935.559	162909	(e)	11/2	269797	(0)	9/2	4.46E09	3.02E09	-0.22	-0.44
937.466	156855	(e)	9/2	263525	(0)	9/2	8.31E08	2.05E09	-0.96	-0.62
937.713	178629	(e)	9/2	285271	(0)	7/2	1.68E08*	7.58E08	-1.64*	-1.04
938.578	170023	(e)	5/2	276567	(0)	7/2	6.32E08	3.89E08	-1.07	-1.34
939.097	168671	(e)	7/2	275157	(0)	7/2	2.93E08	3.17E07#	-1.40	-2.42#
940.328	163804	(e)	13/2	270150	(0)	11/2	3.36E08	3.96E08	-1.34	-1.32
940.775	167125	(e)	9/2	273421	(0)	7/2	1.00E09	2.57E09	-0.88	-0.52
941.636	167223	(e)	5/2	273421	(0)	7/2	1.88E09	1.14E09	-0.60	-0.87
947.805	151786	(e)	13/2	257293	(0)	13/2	9.74E09	1.03E10	0.12	0.09
948.762	158125	(e)	11/2	263525	(0)	9/2	1.64E09	2.83E09	-0.65	-0.47
950.032	170023	(e)	5/2	275283	(0)	5/2	1.28E09	3.95E08	-0.76	-1.33
950.246	180036	(e)	7/2	285271	(0)	7/2	4.67E08	5.21E09	-1.19	-0.19
950 729	162806	(e)	9/2	267988	(0)	11/2	7 93E07*	5 22E08	-1 97*	-1.20
951 237	162806	(e)	9/2	267932	(0)	9/2	4 63E07*	1 42E09	-2 20*	-0.76
951.662	162909	(e)	11/2	267988	(0)	11/2	1.65E09	4 43E09	-0.64	-0.26
052 173	162909	(c) (e)	11/2	267932	(0)	0/2	2 05E08*	1.43E09	1 55*	0.20
052.175	186818	(\mathbf{c})	5/2	201952	(0)	5/2	2.05108	2 80E00	-1.55	-0.70
952.075	196919	(e)	5/2	291704	(0)	2/2	2.70E09	2.80E09	-0.44	-0.48
933.103 054 274	100010	(\mathbf{c})	512 12/2	271133 256566	(0)	51Z 11/2	1.JOEU9 5 /0E00	1.4JEU9 5 57E00	-0.08	-0.77
yJ4.J/4 056 772	131/80	(e)	13/2	230300 275157	(0)	11/2	J.47EU7 0 14E07*	J.J/EU9	-0.13 1.04*	-0.17
930.772 059.070	171005	(e)	912 510	2/313/	(0)	112 5 12	0.14EU/*	1.22EU9	-1.94* 1.50	-0.82
958.970	1/1005	(e)	512	213283	(0)	512	2.1/EU8	1.19E09	-1.52	-0.84
960.921	1/3520	(e)	112	277587	(0)	5/2	1.93E09	2.36E09	-0.57	-0.54
963.227	1/1465	(e)	3/2	275283	(0)	5/2	9.93E08	1.33E09	-0.86	-0.79
965.653	166240	(e)	9/2	269797	(0)	9/2	7.30E08	1.13E09	-0.98	-0.85
974.890	189188	(e)	7/2	291764	(0)	5/2	9.79E08	5.43E08	-0.85	-1.16
	197304	(e)	13/2	299879	(0)	11/2	5.16E09	4.92E09	-0.13	-0.19
978.015	197304	(e)	13/2	299551	(0)	13/2	8.87E09	9.56E09	0.11	0.10
979.306	171307	(e)	7/2	273421	(0)	7/2	1.44E09	1.22E09	-0.68	-0.80

1002.891

156855

9/2

(e)

256566

11/2

(0)

7.45E08

-0.95

8.86E08

-0.92

	Lower leve	el ^b		Unner leve	1 ^b		$\sigma A (s^{-1})^c$		log of ^c	
Wavelength $(\text{\AA})^a$	$E(cm^{-1})$	(P)	I	$E(cm^{-1})$	(P)	T	HFR^d	$MCDHF^{e}$	HFR^d	$MCDHF^{e}$
1008 394	158125	(r) (e)	11/2	257293	(1)	13/2	6 14F08	6 54F08	-1 03	-1.05
1015 829	158125	(c) (e)	11/2	257275	(0)	11/2	5 73E08	6.75E08	-1.05	-1.03
1236 607	187526	(c) (e)	15/2	250500	(0)	15/2	1 76E04*	9 56E03#	-5.38*	-5.68#
1247 456	217147	(c) (e)	13/2	200373	(0)	0/2	1.70L04	1 30E07	-5.50	2.00#
1247.430	21/14/	(e)	7/2	297310	(0)	212 CIT	1.10E07* 2.83E07*	1.39E07 5.16E05#	-2.57	-2.40
1420 023	207779	(\mathbf{c})	11/2	203271	(0)	13/2	5 36E00	5.00E00	-2.13	-5.88
1420.023	243332	(e)	0/2	287200	(0)	1312	J.J0E09	3.60E09	0.23 2.81*	0.18
1429.209	243530	(\mathbf{c})	13/2	207390	(0)	11/2	4.90L00	$2.02E04\pi$	-2.01	-4.90#
1452.500	243339	(e)	13/2	277587	(0)	5/2	2.31E09	2.15E09	-0.09	-0.18
1422 771	201119	(e)	11/2	212247	(0)	11/2	1.76E09	2.49E09	-0.20	-0.12
1432.771	243332	(e)	5/2	200642	(0)	11/2	1.40E10 2.21E00	1.34E10	0.07	0.07
1455.550	210902	(e)	$\frac{3/2}{11/2}$	200042	(0)	11/2	2.21E09	1.21E09	-0.15	-0.43
1441.701	211937	(e)	0/2	201510	(0)	11/2	1.12E10 4.50E07*	1.14E10 1.61E00	0.30	0.30
1441.952	207210	(e)	9/2	2/030/	(0)	11/2	4.50E07*	1.01E09	-1.83*	-0.29
1445.041	212047	(e)	912	281310	(0)	0/2	3.37E09	5.10E09	0.20	0.21
1448.158	21/14/	(e)	112 5/2	280201	(0)	912 510	3.40E09	4.3/E09	0.00	0.14
1449.324	218982	(e)	5/2	287980	(0)	5/2	2.93E08	3.94E04#	-1.02	-4.90#
1450.356	201310	(e)	11/2	270258	(0)	13/2	6.31E09	3.27E09	0.32	0.02
1450.686	228377	(e)	11/2	29/310	(0)	9/2	5.15E09	4.96E09	0.23	0.20
1452.469	211957	(e)	11/2	280805	(0)	9/2	2.51E09	2.19E09	-0.08	-0.15
1452.638	201310	(e)	11/2	2/0150	(0)	11/2	7.11E09	6.2/E09	0.37	0.30
1453.353	219261	(e)	7/2	288068	(0)	9/2	1.33E10	1.30E10	0.64	0.62
1453.751	207779	(e)	7/2	2/656/	(0)	112	9.94E08	4.73E09	-0.50	0.18
1453.910	217422	(e)	9/2	286201	(0)	9/2	5.42E09	7.26E09	0.25	0.37
1454.375	212047	(e)	9/2	280805	(0)	9/2	1.09E10	1.09E10	0.56	0.55
1455.214	207216	(e)	9/2	275935	(0)	11/2	1.47E09	1.57E10	-0.30	0.70
	219261	(e)	7/2	287980	(0)	5/2	7.04E08	8.94E07	-0.63	-1.55
1459.156	217422	(e)	9/2	285954	(0)	7/2	1.96E07*	2.06E09	-2.19*	-0.17
1460.113	201310	(e)	11/2	269797	(0)	9/2	3.64E09	4.63E09	0.08	0.18
1460.708	220182	(e)	5/2	288642	(0)	7/2	8.12E09	9.14E09	0.43	0.47
1461.825	218982	(e)	5/2	287390	(0)	7/2	4.63E09	4.81E09	0.19	0.20
1463.514	228377	(e)	7/2	296706	(0)	7/2	8.58E09	8.47E09	0.46	0.44
1464.031	218982	(e)	5/2	287287	(0)	5/2	4.67E09	5.23E09	0.20	0.23
1467.809	219261	(e)	7/2	287390	(0)	7/2	5.60E09	5.44E09	0.28	0.25
1468.749	202173	(e)	11/2	270258	(0)	13/2	1.24E08	2.72E09	-1.37	-0.05
	219202	(e)	3/2	287287	(0)	5/2	1.91E09	5.06E08	-0.19	-0.77
1468.991	217422	(e)	9/2	285495	(0)	11/2	1.62E10	1.56E10	0.74	0.71
1469.454	212047	(e)	9/2	280099	(0)	7/2	8.76E09	7.78E09	0.47	0.41
1470.045	219261	(e)	7/2	287287	(0)	5/2	1.39E09	1.96E09	-0.33	-0.19
1471.094	202173	(e)	11/2	270150	(0)	11/2	1.37E08	5.31E09	-1.32	0.24
1471.203	228554	(e)	9/2	296526	(0)	11/2	1.60E10	1.56E10	0.73	0.71
1471.880	207216	(e)	9/2	275157	(0)	7/2	1.92E08	1.14E09	-1.19	-0.43
1472.120	207779	(e)	7/2	275709	(0)	9/2	3.56E09	5.14E09	0.08	0.23
1473.710	211957	(e)	11/2	279813	(0)	13/2	1.89E10	1.82E10	0.81	0.78
1475.774	217147	(e)	7/2	284908	(0)	5/2	7.15E09	6.85E09	0.39	0.36
1478.758	202173	(e)	11/2	269797	(0)	9/2	4.89E07*	3.81E09	-1.77*	0.10
1484.176	207779	(e)	7/2	275157	(0)	7/2	6.76E09	2.95E09	0.36	-0.01
1485.582	243539	(e)	13/2	310853	(0)	15/2	2.13E10	2.07E10	0.87	0.85
1487.908	220182	(e)	5/2	287390	(0)	7/2	5.69E08	2.65E08	-0.70	-1.04
1493.883	219261	(e)	7/2	286201	(0)	9/2	1.61E08	1.52E08	-1.25	-1.28
1499.728	201310	(e)	11/2	267988	(0)	11/2	6.00E09	9.72E08	0.31	-0.48
1500.734	207779	(e)	7/2	274413	(0)	5/2	6.23E09	5.47E09	0.33	0.27
1500.995	201310	(e)	11/2	267932	(0)	9/2	8.65E09	1.55E09	0.47	-0.28
1510.946	207216	(e)	9/2	273400	(0)	9/2	3.22E08	8.63E08	-0.95	-0.52
1516.850	218982	(e)	5/2	284908	(0)	5/2	2.62E08	1.72E08	-1.02	-1.20
1519.401	202173	(e)	11/2	267988	(0)	11/2	1.64E08	9.52E08	-1.23	-0.48
1520.695	202173	(e)	11/2	267932	(0)	9/2	2.13E08	1.49E09	-1.12	-0.29
1523.901	207779	(e)	7/2	273400	(0)	9/2	2.22E09	5.29E08	-0.11	-0.70
1536.335	220182	(e)	5/2	285271	(0)	7/2	2.30E08	5.68E07	-1.07	-1.67
1544.949	220182	(e)	5/2	284908	(0)	5/2	2.23E08	3.47E08	-1.07	-0.88

7/2

(0)

3.00E08

1.32E09

-0.93

-0.31

1584.538

212047

9/2

(e)

275157

	Lower leve	el^b		Upper leve	el^b		$gA(s^{-1})^{c}$		$\log gf^c$	
Wavelength $(Å)^a$	$E(cm^{-1})$	(P)	J	$E(cm^{-1})$	(P)	J	\mathbf{HFR}^{d}	MCDHF^{e}	HFR^d	MCDHF^{e}
1629.368	212047	(e)	9/2	273421	(0)	7/2	4.62E08	6.28E08	-0.73	-0.61
1647.007	207216	(e)	9/2	267932	(0)	9/2	2.44E07	2.06E08	-1.99	-1.06
1677.768	228377	(e)	7/2	288068	(0)	9/2	4.85E07*	4.61E07	-1.68*	-1.76
1709.023	217422	(e)	9/2	275935	(0)	11/2	2.58E07*	5.81E07	-1.92*	-1.59
1721.095	212047	(e)	9/2	270150	(0)	11/2	3.16E09	1.03E09	0.17	-0.33
1723.849	217147	(e)	7/2	275157	(0)	7/2	3.35E07*	7.94E07	-1.81*	-1.45
1728.896	211957	(e)	11/2	269797	(0)	9/2	4.86E09	1.94E09	0.36	-0.05
1731.593	212047	(e)	9/2	269797	(0)	9/2	1.15E09	4.77E08	-0.27	-0.66
1736.574	218982	(e)	5/2	276567	(0)	7/2	1.75E09	9.55E08	-0.08	-0.35
1741.985	220182	(e)	5/2	277587	(0)	5/2	1.45E09	1.37E09	-0.17	-0.19
1757.639	228377	(e)	7/2	285271	(0)	7/2	3.70E07*	1.25E09	-1.76*	-0.24
1760.697	200497	(e)	13/2	257293	(0)	13/2	3.79E09	3.50E09	0.25	0.21
1773.513	220182	(e)	5/2	276567	(0)	7/2	9.71E08	3.47E08	-0.32	-0.76
1775.340	243552	(e)	11/2	299879	(0)	11/2	1.23E09	1.06E09	-0.23	-0.30
1775.921	207216	(e)	9/2	263525	(0)	9/2	3.22E08	2.93E09	-0.81	0.15
1776.176	218982	(e)	5/2	275283	(0)	5/2	1.50E09	1.38E09	-0.15	-0.18
1777.040	217147	(e)	7/2	273421	(0)	7/2	1.32E09	1.16E09	-0.20	-0.26
1777.677	217147	(e)	7/2	273400	(0)	9/2	2.83E09	4.10E09	0.13	0.29
1780.161	218982	(e)	5/2	275157	(0)	7/2	2.21E08	1.13E09	-0.96	-0.25
1783.126	219202	(e)	3/2	275283	(0)	5/2	2.64E08	1.46E08#	-0.90	-1.15#
1783.513	200497	(e)	13/2	256566	(0)	11/2	8.14E09	7.86E09	0.59	0.58
1784.713	211957	(e)	11/2	267988	(0)	11/2	1.58E09	2.36E09	-0.12	0.06
1785.034	219261	(e)	7/2	275283	(0)	5/2	2.81E09	2.83E09	0.13	0.13
1785.199	228377	(e)	7/2	284393	(0)	9/2	3.13E09	4.04E09	0.18	0.29
1785.749	243552	(e)	11/2	299551	(0)	13/2	8.61E09	8.45E09	0.61	0.60
	217422	(e)	9/2	273421	(0)	7/2	4.48E09	4.18E09	0.33	0.30
1786.254	201310	(e)	11/2	257293	(0)	13/2	7.43E09	3.98E09	0.55	0.28
1786.411	217422	(e)	9/2	273400	(0)	9/2	1.91E09	2.45E09	-0.04	0.07
1786.501	211957	(e)	11/2	267932	(0)	9/2	1.81E09	4.46E09	-0.05	0.33
1787.584	212047	(e)	9/2	267988	(0)	11/2	3.44E09	5.29E09	0.22	0.41
1789.384	212047	(e)	9/2	267932	(0)	9/2	3.13E08	8.20E08	-0.81	-0.40
1789.056	219261	(e)	7/2	275157	(0)	7/2	1.66E08	9.00E08	-1.08	-0.35
1790.865	228554	(e)	9/2	284393	(0)	9/2	2.01E09	2.46E09	-0.01	0.08
1793.854	207779	(e)	7/2	263525	(0)	9/2	4.22E09	3.84E09	0.31	0.27
1800.399	207779	(e)	7/2	263323	(0)	7/2	1.59E09	1.52E09	-0.11	-0.13
1809.730	201310	(e)	11/2	256566	(0)	11/2	1.49E09	7.05E08	-0.13	-0.46
1811.205	219202	(e)	3/2	274413	(0)	5/2	5.02E08	6.33E08	-0.58	-0.48
1814.240	202173	(e)	11/2	257293	(0)	13/2	1.42E08	3.30E09	-1.14	0.21
1819.006	220182	(e)	5/2	275157	(0)	7/2	2.80E07	1.53E08	-1.83	-1.09
1838.460	202173	(e)	11/2	256566	(0)	11/2	3.49E07	6.11E08	-1.74	-0.51
1843.938	220182	(e)	5/2	274413	(0)	5/2	3.05E08	4.34E08	-0.78	-0.63

^a Experimental wavelengths measured by Kaufman and Sugar (1978) and Ryabtsev et al. (2015)

^b Lower and upper levels of the transitions are represented by their experimental values (in cm⁻¹), their parities ((e) for even and (o) for odd) and their J-values. Level energies (rounded values), are taken from Kaufman and Sugar (1978) and Ryabtsev et al. (2015)

^c Weighted transition probabilities (gA) and oscillator strengths $(\log(gf))$ calculated using HFR method (this work)

^d gA- and $\log(gf)$ -values with the * symbol correspond to transitions for which CF < 0.05 in HFR calculations (this work)

^e gA- and $\log(gf)$ -values with the # symbol correspond to transitions for which dT > 0.20 in the MCDHF calculations (this work)