

# Poster Contributions

Laboratory Data (LD)

Theory and Calculations (TC)

Laboratory Plasmas and Experiments (LPE)

Astrophysical Plasmas (AP)

Databases and Data Assessment (DBA)



## Laser spectroscopy of the Zeeman-hf structure of atomic niobium

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The hyperfine and Zeeman structures of 36 lines of Nb I covering the 573.7-649.4 nm spectral region have been measured [1,2]. We used three techniques of laser spectroscopy: optogalvanic spectroscopy (OG), laser induced fluorescence (LIF) and fluorescence depletion spectroscopy (FDS). The source of free niobium atoms was a hollow cathode discharge lamp. In spectral analysis, we used software that takes into account the saturation effect. One of the measured structure and their computer analysis is presented in the figure below.

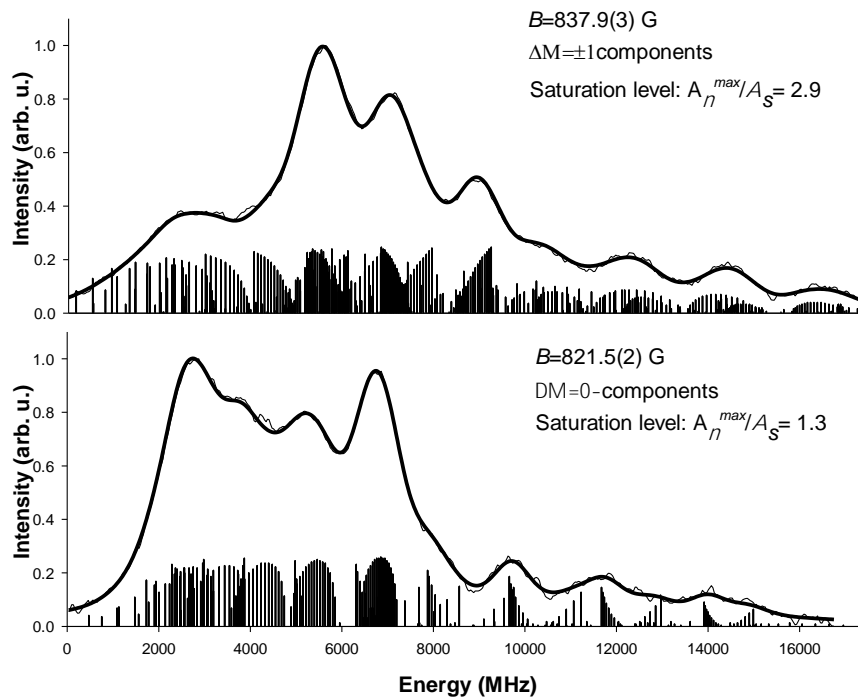


Figure 1: FDS spectra of the Zeeman-hf structures ( $\pi$  and  $\sigma$  patterns) of the 586.493 nm line in the magnetic field above 800 G. The computer generated profiles (thick lines) take into account the saturation effect. As it can be seen the saturation effect appears and the ratio for the  $M, M'$  component of the highest intensity  $A_v^{max}$  to the saturation rate  $A_S$  equals 2.9 and 1.3 for  $\Delta M = \pm 1$  and  $\Delta M = 0$  components, respectively.

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## **New experimental energy levels, lifetimes and oscillator strengths in singly ionised zirconium**

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Recent advances in resolution and spectral range of ground-based and space-based astronomical spectrographs, call for accurate atomic data in order to reliably interpret and model astrophysical spectra. Correctly interpreted, stellar spectra allow for precise abundance analysis which, in turn, makes it possible to study the Galactic formation and evolution. To meet this demand, we study the complex atomic system of singly ionised zirconium, Zr II. Zirconium is predominantly found in cool giants and sub-dwarfs, as well as in kilonova spectra, providing a way to study the s-process and r-process elements.

In this project we report completely new experimental energies for 20 highly excited states belonging to the  $4d^26s$  and  $4d^25d$  configurations in Zr II. We have also measured radiative lifetimes for these levels, and combined with branching fractions we have derived experimental transition probabilities (oscillator strengths) for 104 lines between the first odd  $4d^25p$  and  $4d5s5p$  configurations and the new levels. The energy levels were identified from lines in spectra recorded with a Chelsea Instruments FT500 Fourier transform spectrometer, using a hollow cathode as light source, and the branching fractions were measured in the same intensity calibrated spectra. The lifetimes were measured with a laser induced fluorescence technique at the Lund Laser Centre.

## THE SPECTRUM AND ENERGY LEVELS OF DOUBLY IONISED NEODYMIUM

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Radiative properties of the neutral, singly, and doubly ionized rare-earth element neodymium ( $Z = 60$ ) are of astrophysical interest, particularly in the spectra of chemically peculiar stars [1] and kilonovae of neutron star mergers [2,3]. Experimentally, little is known of the atomic structure of doubly ionised neodymium (Nd III), only 40 energy levels were previously published [1]. Using the Imperial College VUV Fourier transform spectrometer, intensity and wavenumber calibrated spectra of a pure Nd cathode Penning discharge lamp were recorded in the region  $11500\text{-}54000\text{ cm}^{-1}$  ( $8695\text{-}1852\text{ \AA}$ ) at resolving powers of up to  $10^6$ . Fourier transform spectra of Nd hollow cathode discharges, Nd vacuum spark grating spectra, and UVES stellar spectra were used to aid the line and energy level classification of lower-lying levels of the  $4f^4$ ,  $4f^35d$ ,  $4f^36s$ ,  $4f^36p$ ,  $4f^37s$ , and  $4f^36d$  configurations. New and more accurate semi-empirical calculations were made using the Cowan code for these configurations. In total, 184 energy levels and 570 transitions of Nd III have been classified and measured with accuracies up to a few parts in  $10^8$ , the classified transitions are presented in Figure 1. Analysis of the  $4f^35f$  configuration by grating spectroscopy is ongoing, from which an additional 68 levels have been classified so far.

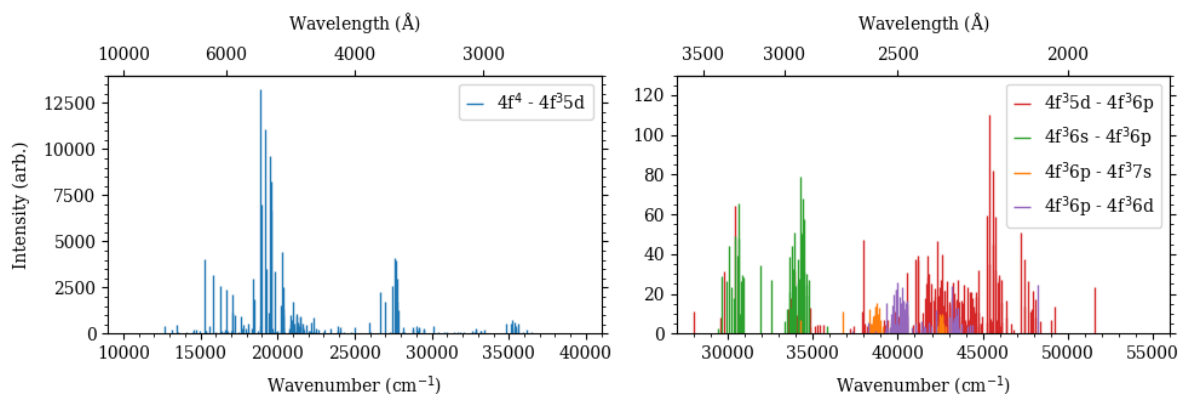


Figure 1: Classified Nd III lines from the Penning discharge lamp spectra. Three lines of the  $4f^4 - 4f^36s$  transitions were also observed (not shown). The two intensity scales are the same.

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This work is supported by the STFC of the UK and the research project FFUU-2022-0005 of the Institute of Spectroscopy of the Russian Academy of Sciences.

## REVISED ENERGY LEVELS OF ATOMIC HOLMIUM CONSIDERING HYPERFINE STRUCTURE IN FOURIER TRANSFORM SPECTRA

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Holmium (Ho) is the fifth to last element in the series of lanthanides. The atomic spectrum of Ho is characterized by a broad hyperfine structure (hfs) of the only stable isotope, <sup>165</sup>Ho, which has a nuclear spin of  $I = 7/2$ , a large nuclear magnetic dipole moment as well as a large electric quadrupole moment. As a result, the hfs of most spectral lines of the Ho atoms and ions can be resolved using Doppler-limited spectroscopic methods such as Fourier spectroscopy.

Numerous studies of fine and hyperfine structure have been carried out in recent years (of which only the most recent publications are listed here, see [1-4] and citations therein). Several of these previous papers have revealed large uncertainties in the energy values of the fine structure levels of atomic Ho.

In this study, revised values for the fine structure level energies of atomic Ho are presented. Based on the experimental wavenumbers of more than 1400 spectral lines from calibrated Fourier transform (FT) spectra, the energy of fine structure levels of atomic Ho has been revised by weighted global fits. Various spectroscopic techniques have previously been used by different researchers and also our group to classify the Ho spectral lines before and to provide data for the hfs constants. The line classifications have been reviewed and for the high accurate determination of the center of gravity wavenumbers from the FT spectra, the hfs constants of the involved levels have been taken into account.

When checking the classification, each spectral line was assigned a weighting factor depending on its intensity in the spectrum, whether its hfs is well resolved or not, and whether it is blended with other lines. Based on these data, an overdetermined linear equation system was built up. Subsequently the revised energy levels were obtained by solving the weighted linear equation system using a self-written GNU Octave script.

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## CHARACTERIZATION OF A HOLLOW-CATHODE LAMP TO MEASURE ACCURATE TRANSITION PROBABILITIES OF RARE-EARTH ELEMENTS

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Rare-earths like neodymium (Nd) have a very wide range of applications. Nd is used, for example, in Nd:YAG LASER and as a dopant in metal-halide high-intensity discharge (MH-HID) lamps, which are more efficient than incandescent lamps [1]. Accurate atomic data of neodymium, such as transition probabilities, are used not only by lighting scientists to model and diagnose MH-HID [2], but also by astrophysicists to calculate chemical abundances of stars [3].

Over the last 30 years, the Atomic Spectroscopy Laboratory at the University of Valladolid (Spain) has reported transition probabilities of noble gases [4]. Due to contemporary needs [5], the laboratory has reopened with the new objective of measuring transition probabilities ( $A_{ki}$ ) of rare-earths. Our aim is to obtain accurate  $A_{ki}$ -values of rare-earths, like Nd, with a hollow-cathode lamp (HCL) and a diffraction grating spectrometer of 150 000 resolving power (at 450 nm) in the UV-visible spectral range. To achieve this goal, the HCL is operated in the abnormal glow region of the carrier gas [6] and it is ensured that the spectra emitted does not vary with time.

In this poster, we will present the voltage-current curve of the lamp also known as the gas discharge characteristic curve of the carrier gas (which is argon in our case) at different pressure inside the lamp to ensure that the lamp is operating in the abnormal glow region. We will also study the stability of the hollow-cathode lamp by studying the variation of line intensities over time. For this, we have measured spectra for a set of selected lines ranging from 300 nm to 700 nm from different upper energy levels for different ionization stages of argon (Ar I, Ar II) and iron (Fe I, Fe II, used as a test cathode) over a period of several hours. We have performed this study under different conditions of pressure and current to analyse the behaviour of the hollow-cathode lamp with different measuring conditions

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# A JOINT THEORETICAL AND EXPERIMENTAL APPROACH TO DIELECTRONIC RECOMBINATION DATA FOR PHOTOIONIZED ASTROPHYSICAL ENVIRONMENTS

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Uncertainties in dielectronic recombination (DR) rate coefficients that are used in current modeling and diagnostic codes represent a obstacle for the accurate determination of elemental and charge state abundances of low-temperature astrophysical plasmas. This in turn has an impact on cosmological models of elemental abundances and evolution. Accurate data for low temperature DR remains sparse from experiments, while theoretical rates have large uncertainties due to the difficulty in calculating many-body effects for low-energy resonances, particularly for elements beyond the second row of the periodic table. These same theoretical uncertainties also contribute to uncertainties in DR satellite line wavelengths and intensities. The new DR data generated as a part of the proposed project will have an impact on the study of several areas of astronomy, e.g., galaxy evolution, H II regions, gas-rich dwarfs and planetary nebulae.

In this work, we address the issue of low temperature DR rate coefficients for astrophysical photoionized plasmas, where the DR rates are known to have large uncertainties in their calculated values. A commonly used code for computing DR rates is AUTOSTRUCTURE, which uses the multi-configuration Breit-Pauli approach. The current approach makes use of large configuration-interaction (CI) calculation using the AUTOSTRUCTURE code. Although effective in the high temperature case, current theoretical methods are known to have large uncertainties in the low temperature regime due to uncertainties in calculating low-*n* doubly excited states. This can be observed via comparison with ion storage ring measurements. We have developed an algorithmic method for the generation of large configuration sets to improve the low temperature DR modeling through CI. These new theoretical DR rate coefficients are then compared to existing storage ring measurements and will also be compared to new measurements being performed at the heavy ion storage ring CRYRING@ESR at the FAIR facility in Darmstadt, Germany.

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## EXTENDED ANALYSIS OF THE VUV EMISSION SPECTRUM OF THE FREE ION Er<sup>+2</sup> (Er III)

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Lanthanides have multiple applications, notably in astrophysics and in photonics. The complexity of their spectra implies a systematic study by isoelectronic or isoionic sequences. The first study of the spectrum of the Er<sup>+2</sup> ion, concerning the 5p<sup>6</sup>4f<sup>12</sup>, 4f<sup>11</sup>5d, 4f<sup>11</sup>6s and 4f<sup>11</sup>6p configurations by Nissan Spector [1] was summarized in the NBS critical compilation in 1978 [2]. An extended study of these configurations in Er<sup>+2</sup> ion was taken up by Wyart et al [3], and led to increase the number of known energy levels from 45 to 115, and to identify 470 new spectral lines in the spectral range between 2000 and 7000Å. Our objective is to further extend the analysis of this spectrum to the VUV wavelength region below 2000Å, where identification of new spectral lines could allow the determination of higher energy levels. The analysis is based on the VUV emission spectrum of erbium produced in the spectral region of 705-2460 Å, already used for the Er IV analysis [4,5]. All the spectrograms have been recorded on photographic plates (PP) or image plates (IP), using the high-resolution normal incidence spectrograph at Meudon Observatory with a vacuum spark emission source.

Theoretical predictions of energy levels and transition probabilities were carried out by means of Cowan codes (RCN, RCG, and RCE) with relativistic corrections (HFR option) [6]. Configuration interactions were investigated in the calculations, including in the even parity (5p<sup>6</sup>4f<sup>12</sup>, 4f<sup>11</sup> 6p, 4f<sup>10</sup>5d<sup>2</sup>, 4d<sup>10</sup>5d6s, 4f<sup>11</sup>5f and 5p<sup>5</sup>4f<sup>13</sup>) and in the odd parity, (4f<sup>11</sup>5d, 4f<sup>11</sup>6s, 4f<sup>11</sup>6d, 4f<sup>11</sup>7s, 5p<sup>5</sup>4f<sup>12</sup>5d and 5p<sup>5</sup>4f<sup>12</sup>6s). The parameters calculated at the HFR step were corrected with scaling factors of the Tm<sup>+3</sup> [7] and Yb<sup>+4</sup> [8] ions when available, which allowed us to improve the initial predictions of energies and transition probabilities. Results on spectral line identifications and new energy levels will be presented, together with parametric fits of energy parameters.

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**ENERGY LEVELS AND TRANSITION DATA OF Au IV**

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In this contribution, reliable atomic data for triply ionized gold (Au IV) were presented with the help of its spectrum investigated in the wavelength region of 500–2106 Å. The spectra of gold were photographed on 10.7-m normal incidence vacuum spectrograph using a sliding spark source at the National Institute of Standards and Technology (NIST, USA) as well as on a 3-m NIVS at the Antigonish laboratory in Canada with a triggered spark source. A total of 139 energy levels of Au IV were established with the help of 1031 classified transitions. The theoretical support for the present observations was made with the use of extended Cowan's codes (HFR) calculations for Au IV and HFR+CPOL (core-polarization effects). Several astrophysically relevant transitions, forbidden (M1- and E2-type) transitions of  $5d^8$  and  $5d^76s$  configurations are provided with their Ritz wavelengths and radiative parameters. The transition data for forbidden types were computed within the frameworks of HFR, HFR+CPOL and GRASP2K codes. A critically evaluated set of the Au IV's energy levels, observed and Ritz wavelengths along with their uncertainties, and transition rates were presented.

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## DOUBLY-IONISED IRON : NEW ACCURATE WAVELENGTHS AND ENERGY LEVELS

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Presented here is new laboratory-measured doubly-ionised iron (Fe III) transition wavelengths and energy level values, to meet the need for higher quality atomic data. These data will be invaluable to astronomers as the spectral lines of iron are present in, and dominate opacities of, many astrophysical sources, due to its complex spectrum and high relative abundance.

Fe III spectra were generated using a Penning discharge lamp (PDL) and recorded on the high-resolution vacuum-ultraviolet (VUV) Fourier transform (FT) spectrometer at Imperial College (IC) London, UK. This instrument has a resolving power of up to  $\sim 2$  million at 200 nm, resulting in the most accurate Fe III linelist produced to date in the UV-VUV (152.7 nm to 295.6 nm). The strongest Fe III spectral lines recorded had uncertainties between 0.000027 nm and 0.00012 nm.

As our FT spectrometer has a lower wavelength limit of  $\sim 135$  nm, these accurate wavenumbers were supplemented with grating spectra in the lower wavelength region. The grating spectra (90 nm to 181 nm) were recorded on the 10.7 m normal incidence vacuum spectrograph (NIVS) at the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, USA. Both the FT and grating spectra were wavenumber calibrated using Fe II Ritz wavelengths published by [1]. The FT data were calibrated to an accuracy of 5 - 8.5 parts per  $10^8$ .

Using the observed transition wavelengths, an extensive term analysis of the lower-lying energy levels of Fe III has been conducted. The results include the revision of 313 previously published atomic energy level values and 1890 Ritz wavenumbers identified as Fe III transitions in the UV-VUV, which are at least an order-of-magnitude more accurate than previous publications. The atomic data reported here have numerous applications in astronomy. These accurate Fe III transition wavelengths will be used as wavelength standards to calibrate VUV spectra of hot stars and for the identification of spectral lines.

Additionally, 400 parity-forbidden Fe III Ritz wavelengths have been calculated between the lowest-lying configurations,  $3d^6$  and  $3d^5(ML)4s$ . These findings will assist astronomers in analysing spectra obtained from diluted astrophysical plasmas.

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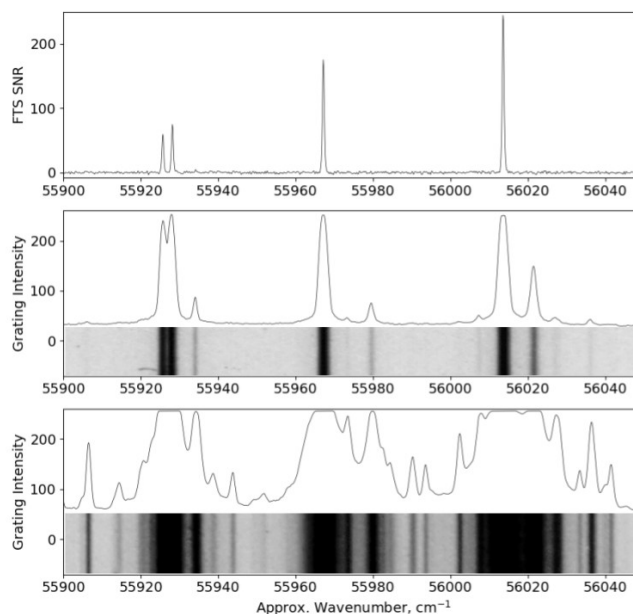


Figure 1: The iron spectrum observed on the IC FT spectrometer [top], and on the NIST NIVS with 5-minute [middle] and 45-minute exposure [bottom].

## Multiplatform determination of the radiative properties of the seventh spectrum of tantalum (Ta VII)

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Tantalum ( $Z=73$ ) is an element that is produced in the neutron-induced transmutation of tungsten ( $Z=74$ ) which in turn will compose the divertors in Tokamaks [1]. As a consequence, their sputtering may generate ionic impurities of all possible charge states in the deuterium-tritium plasma that could contribute to radiation losses in controlled nuclear devices. The radiative properties of these ions have therefore potential important applications in this field.

In this context, a multiplatform approach has been adopted in order to compute the Ta VII radiative rates and estimate their accuracy. The oscillator strengths and transition probabilities have been calculated for the 237 E1 transitions in Ta VII as classified in 2014 by Ryabtsev *et al* [2]. Three independent atomic structure models have been used; one based on the semi-empirical pseudo-relativistic Hartree-Fock (HFR) method [3] and two based on the fully relativistic *ab initio* multiconfiguration Dirac-Hartree-Fock (MCDHF) method [4,5].

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# JAC: A community platform for just atomic computations

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Electronic structure calculations of atoms and ions have a long tradition in physics with applications in basic research and spectroscopy. With the Jena Atomic Calculator (JAC), I here present a new implementation of a (relativistic) electronic structure code for the computation of atomic amplitudes, properties as well as a large number of excitation and decay processes for open-shell atoms and ions across the periodic table. JAC [1] is based on Julia, a new programming language for scientific computing, and provides an easy-to-use but powerful platform to extent atomic theory towards new applications.

A primary guiding philosophy in designing JAC was to develop a general and easy-to-use toolbox for the atomic physics community, including an interface that is equally accessible for working spectroscopists, theoreticians and code developers. In addition, I also wish to provide a modern code design, a reasonable detailed documentation of the code and features for integrated testing [2].



Figure 1: Overview of the JAC toolbox.

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# THEORETICAL STUDY OF SPECTRA OF Hf VI USING A MULTIPLATFORM APPROACH

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Hafnium ( $Z = 72$ ) is an element that could be employed in plasma-facing materials in Tokamaks [1,2] and is also produced in neutron-induced transmutation of tungsten ( $Z = 74$ ) and its alloys that will compose the divertors in these fusion reactors [3]. As a consequence, their sputtering may generate ionic impurities of all possible charge states in the deuterium-tritium plasma. These impurities could contribute to radiation losses in controlled nuclear fusion devices. The radiative properties of these ions have therefore potential important applications in this field [4,5,6].

**Many lines of Hf VI in UV range, precisely from 193 Å to 474 Å, have been calculated. As no experimental determination of radiative rates is available in the literature, a multiplatform approach has been adopted to carry out the present calculations so as to estimate the accuracy of the computed rates.**

From the comparisons of our three independent models based on both the HFR [7] and MCDHF [8,9] methods along with the calculations published by Ryabtsev et al. [5] that they used for line classification purpose, it was found that the uncertainties affecting the theoretical rates range from a few percent (for our HFR model) to ~40 % (for our MCDHF-RCI-A model) for the strong E1 transitions with  $S \geq 1$  a.u. With respect to the other lines, they can be highly inaccurate with uncertainties far more than 100 % due to strong cancellation effects and important gauge disagreements that render the rates highly model sensitive. This is essentially caused by the strong mixing affecting most of the Hf VI atomic states. **Finally, we recommend our HFR rates except for the two lines at 223.172 Å and at 231.451 Å where the  $gA$ -values of Ryabtsev et al. [5] should be used instead with an uncertainty indicator *Unc.* equal to E (> 50 %), due to strong cancellation effects affecting the former for these two transitions.**

We have plotted in 3 figures the difference between the level energy calculated in our three independent models and the one determined experimentally by Ryabtsev et al [5]; also plotted in 3 figures the comparison of our transition probabilities, with respect to the calculation of Ryabtsev et al. [5], The ratio,  $gA_{HFR}/gA_{RYA}$ , is plotted versus our HFR line strength,  $S_{HFR}$ , both in logarithmic scale. Similar plots are displayed for our MCDHF-RCI-A and our MCDHF-RCI-B models.

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## The effect of electron correlation on trielectronic recombination rate coefficients for Be-like argon

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The merged-beam rate coefficients of dielectronic and trielectronic recombinations (DR and TR) within  $\Delta N = 0$  channels for Be-like Ar14+ were measured by Huang et al. [Astrophys. J. Supp. Ser. 235, 2 (2018)] with the cooler storage ring at Lanzhou, China. Meanwhile, theoretical data were also calculated with AUTOSTRUCTURE (AS) code for comparison with the measured resonance spectrum. However, the AS calculations in most cases significantly underestimated TR resonance strengths. In the present work, we find that the electron correlation between DR and TR resonance states with different captured electron principal quantum numbers  $n$  can lead to an obvious enhancement in TR resonance strengths, which is cross-validated via the relativistic distorted-wave (RDW) approximation implemented in the Flexible Atomic Code (FAC) and the semi-relativistic distortedwave (SRDW) approximation implemented in the AS code. Previous theoretical calculations for this system, however, did not include this form of electron correlation.

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## **THE FINGERPRINTS OF PERIODIC ELECTRIC FIELDS ON LINE SHAPES EMITTED IN PLASMAS**

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Periodic electric fields are found in many kinds of plasmas and result from the presence of collective fields amplified by plasma instabilities, or are created by external sources such as microwave generators or lasers. Spectral lines emitted by atoms or ions in a plasma exhibit a frequency profile characteristic of plasma conditions such as the temperature and density of charged particles. The fingerprints of periodic electric fields appear clearly on the line shape for a large range of frequencies and magnitudes of the oscillating electric field. Satellite structures appear near to multiples of the oscillation frequency and redistribute the intensity of the line far from the line center. The modeling of the simultaneous effects of the plasma microfield and of a periodic electric field has been active since the seventies, but remains difficult to be done accurately since the quantum emitter is submitted to several time dependent electric fields, each with its own characteristic time. We describe here a numerical approach which couples a simulation of the motion of charged plasma particles with an integration of the emitter Schrödinger equation. Resulting line shapes are presented for different plasmas and periodic fields encountered in laboratory and astrophysical plasmas.

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## SEMI-EMPIRICAL DETERMINATION OF RADIATIVE PARAMETERS FOR SINGLY IONIZED ATOM OF COBALT

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Cobalt belongs to iron group elements with an open 3d-shell, which structure is interesting in various fields, astrophysics in particular. There is a noticeable interest in determining the overall abundance trend of Co for testing stellar atmosphere models, evaluating galactic chemical evolution and examining the cobalt nucleosynthesis process.

In our earlier works [1, 2] we carried out semi-empirical calculations of the fine and hyperfine structure for both Co II parity configuration systems. In these articles, we made an attempt to resolve significant discrepancies in some experimental results recently published by two research teams [3, 4]. The fine-structure eigenvectors, determined in those studies, were applied in the presented work for the determination of the radiative parameters. Predicting the values of radiative lifetimes and oscillator strengths was the final way to verify the accuracy of the calculated eigenvectors.

The aim of our research is to determine the values of radiative lifetimes and oscillator strengths for Co II based on available experimental data, using a semi-empirical method. A total of 118 values of the oscillator strengths were calculated and compared with the empirical data. Among the lines with small measurement uncertainties, very good agreement was achieved. The largest differences are mainly related to the values specified with an error greater than 20%. The results of our calculations are shown in comparison to experimental data and other theoretical research published by Raassen et al. [5], Quinet et al. [6] and Kurucz [7]. Additionally, lifetime values for 185 levels were calculated, with 34 of them compared to the experimental data. The similarity of our calculated lifetimes to the experimental values indicates good agreement.

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## HYPERFINE SPLITTINGS OF FEW-ELECTRON HELIUMLIKE IONS AND NUCLEAR PROPERTIES

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The hyperfine structures of the  $2^3S$  and  $2^3P$  states of  $7\text{Be}^{2+}$  and  $9\text{Be}^{2+}$  are investigated within the framework of the nonrelativistic quantum electrodynamics (NRQED), including relativistic and radiative corrections up to order  $m\alpha^6$ . The uncertainties of the calculated hyperfine splittings are on the order of tens of ppm, and for  $9\text{Be}^{2+}$  our results improve the previous theoretical and experimental values by at least two orders of magnitude. The improved sensitivity of the hyperfine splittings of  $7,9\text{Be}^{2+}$  to the nuclear Zemach radius and electric quadrupole moment opens the way to future measurements to extract the atomic physics values of these two nuclear properties to an accuracy of 5% or better.

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## Energy and Properties of Sb-like Nd<sup>9+</sup>, P-like, As-like, Sb-like, Bi-like and Mc-like np<sup>3</sup> Atoms and Ions

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The rich energy configuration of multiply ionized atoms offers numerous optical transitions between the ground state and the long-lived excited states. These transitions have numerous practical applications, including identifying and characterizing astronomical objects like stars and galaxies, diagnosing plasma composition, temperature, and density, and serving as frequency standards for precision measurement and testing fundamental constants [1-4]. In this study, we present accurate calculations of the energies and properties of Sb-like Nd<sup>9+</sup> ion and a group of P-like, As-like, Sb-like, Bi-like and Mc-like np<sup>3</sup> atoms and ions (n=3-7), which are useful for making high-accuracy optical clocks as well as for astronomical identification and plasma diagnosis. To achieve this, we used the relativistic multi-reference configuration interaction (MRCI) method under both four-component Dirac-Coulomb all-electron and relativistic effective core potential frameworks, while considering various types of correlation consistent basis sets. Our calculations predicted wavelengths, quality factors, lifetimes, gJ factors, electric quadrupole moment, electric dipole and quadruple polarizabilities, and hyperfine structure constants for Nd<sup>9+</sup> [5] and the np<sup>3</sup> atoms and ions [6], including many previously unmeasured energies and atomic properties. This study also provides a theoretical benchmark for complex multi-valent systems and expands our understanding of astrophysical spectroscopy, plasma diagnosis, and precision measurement based on optical forbidden transitions.

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## Multiconfiguration Dirac-Hartree-Fock calculations of the hyperfine structure in 137-Ba II for the $^2S_{1/2}$ state

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One of the most dominant processes for the creation of heavy elements in our universe is the r-process. In order to explain their abundance, astrophysicists have developed the theory of nucleosynthesis. Most of the nucleosynthesis signatures can be found in the isotopic abundances. This isotopic mixture for the r-process elements can be determined at the stellar surface of r-process enriched stars by measuring the odd-to-even isotopic ratio of these r-process elements [1]. However, the r-process models predict isotopic mixtures that are difficult to constrain observationally because the lines of odd nuclei are affected by hyperfine splitting which can be hard to resolve in a spectrum. If the hyperfine structure can be determined it is thus possible to measure the fraction of the odd-mass isotopes and to relate it to a given nucleosynthetic process. Barium is a r-process element which has a great interest in astrophysics [2]. Its spectrum for different stage of ionization is therefore well known. If one plans to measure the abundance for this element it is therefore crucial to know its hyperfine structure.

In this work, ab initio atomic calculations of the magnetic dipolar hyperfine constant A for the  $5s^25p^66s\ ^2S_{1/2}$  ground state of singly ionized 137-barium were performed. The preliminary results presented here were determined by means of the multiconfiguration Dirac-Hartree-Fock (MCDHF) method [3] with the GRASP2018 code [4]. Three strategies of orbital optimization were used to probe the effect of different electronic correlation effects on the A constant. After that, for each strategy, a series of relativistic configuration interaction calculations (RCI) were carried out by considering other types of correlation effects. Finally, the preliminary results obtained were compared with the experimental value [5] and others theoretical computations [6,7].

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# ALIGNMENT-TRANSFER RATE COEFFICIENTS FOR ELECTRON IMPACT EXCITATION OF O V

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The multipole rate coefficients  $C_0^{KK'}$  for electron impact excitation of ions are required in the analysis of intensity and polarization of lines emitted from non-thermal plasmas with a cylindrically symmetric electron velocity distribution [1]. Among them, the alignment-transfer rate coefficients, corresponding to non-zero even values of  $K$  and  $K'$ , include quantum coherences between magnetic sublevels within the initial and final ion levels, via integration of a linear combination of alignment-transfer  $\sigma_{Q=0}^{KK'}$  and coherence-transfer  $\sigma_{Q\neq 0}^{KK'}$  cross sections [2]. However, the few calculations of the alignment-transfer rate coefficients  $C_0^{KK'}$  published so far consider only the contribution from  $\sigma_{Q=0}^{KK'}$ . This was the case of Ref. [3] where significant discrepancies were observed between theoretical predictions and measurements in the WT-3 tokamak for certain UV lines of Be-like ion O V.

In an attempt to evaluate the effects of coherence-transfer, we report here calculated data of  $C_0^{22}$  for excitations of O V from the metastable levels  $2s2p\ ^3P_1$  and  $^3P_2$  to the  $2s3p$  and  $2p3d$  configuration levels, using the same electron velocity distribution as in [3]. The  $\sigma_{Q=0,\pm 1,\pm 2}^{22}$  cross sections are computed in the relativistic distorted-wave approximation using an extended version [4] of the flexible atomic code. Table 1 gives selected results that illustrate the important contribution of the coherence-transfer cross sections  $\sigma_{Q=\pm 1,\pm 2}^{22}$ , which could be a clue to explain, at least partly, the discrepancies mentioned above.

Table 1: Selected results of  $C_0^{22}$  (in  $\text{cm}^3\text{s}^{-1}$ ) for excitations of O V with and without coherence-transfer.

Excitation	with $\sigma_{Q=\pm 1,\pm 2}^{22}$	without $\sigma_{Q=\pm 1,\pm 2}^{22}$
$2s2p\ ^3P_1 \rightarrow 2s3p\ ^3P_1$	$5.85 \times 10^{-10}$	$1.03 \times 10^{-10}$
$2s2p\ ^3P_2 \rightarrow 2s3p\ ^3P_2$	$5.84 \times 10^{-10}$	$1.04 \times 10^{-10}$
$2s2p\ ^3P_1 \rightarrow 2s3p\ ^3P_2$	$-2.21 \times 10^{-11}$	$-3.00 \times 10^{-12}$
$2s2p\ ^3P_2 \rightarrow 2s3p\ ^3P_1$	$-2.24 \times 10^{-11}$	$-3.18 \times 10^{-12}$

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# CALCULATED OSCILLATOR STRENGTHS FOR SPECTRAL LINES IN Re III-V IONS OF INTEREST TO NUCLEAR FUSION RESEARCH

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It is now well established that tungsten will be one of the main divertor components of the ITER nuclear fusion reactor. When D-T fusion will take place, very energetic neutrons will strike the walls of the reactor and cause the transmutation of tungsten atoms by irradiation. The primary transmutation products for tungsten are rhenium, osmium and tantalum. In particular, the calculations revealed that, after 5-year irradiation under first wall fusion power-plant conditions in ITER, Re, Os and Ta would reach concentrations of 3.8, 1.4, and 0.8 atomic percentage, respectively [1]. As with tungsten, during fusion operations, these atoms, and more particularly rhenium atoms, will be torn from the reactor wall and enter the plasma where they will constitute impurities contributing to the energy loss by radiation but can also be used for plasma temperature and density diagnostics from the analysis of their spectra in all ionization stages. Therefore the radiative properties of these ions have potential important applications in this field. The purpose of the present work is to provide a new set of atomic data (oscillator strengths and transition probabilities) for electric dipole lines in rhenium ions, from Re III to Re V, obtained using two independent theoretical approaches, i.e. the pseudo-relativistic Hartree-Fock method [2] including core-polarization effects (HFR+CPOL) [3,4] and the fully relativistic Dirac-Hartree-Fock (MCDHF) method [5,6].

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# EFFECT OF THE BREIT INTERACTION ON THE ANGULAR DISTRIBUTION OF AUGER ELECTRONS FOLLOWING ELECTRON-IMPACT EXCITATION OF BE-LIKE IONS

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Electron-impact excitation (EIE) of atoms or ions is one of fundamental atomic processes in astrophysical and laboratory plasmas. Chen *et al.* studied the relativistic effect on the angular distribution of Auger electrons following EIE of Be-like ions [1]. However, as a main part of the relativistic effect, the Breit interaction was not considered.

In the present work [2], we studied the angular distribution of Auger electrons following the EIE  $1s^2 2s^2 J=0 \rightarrow 1s 2s^2 2p_{1/2} J=1$  of Be-like  $Mg^{8+}$ ,  $Fe^{22+}$ ,  $Mo^{38+}$ ,  $Nd^{56+}$ ,  $Au^{75+}$ , and  $U^{88+}$  ions using the multi-configurational Dirac-Fock method and the relativistic distorted-wave theory. Special attention was paid to the effect of the Breit interaction on the angular distribution of the emitted Auger electrons. It was found that for low- $Z$  Be-like ions such as  $Mg^{8+}$  the Breit interaction hardly contributes to the angular distribution of the Auger electrons, whereas for medium- and high- $Z$  ions it makes the angular distribution less anisotropic. To be specific, such an effect becomes first more prominent with increasing nuclear charge  $Z$  and, then, less and less when it further increases, as shown in Figure 1 as an example for the impact electron energy of 3.0 times their respective excitation thresholds, where NB and B denote the results without and with consideration of the Breit interaction, respectively.

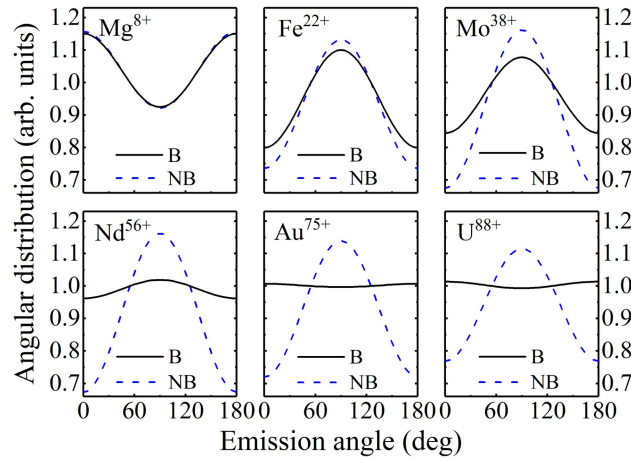


Figure 1: Angular distribution of the Auger electrons emitted from the Auger decay  $1s 2s^2 2p_{1/2} J=1 \rightarrow 1s^2 2s J=1/2$  of Be-like ions for an impact energy of 3.0 times their respective excitation thresholds. Results are given for both NB (blue dashed lines) and B (black solid lines) cases.

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# QUASI-MOLECULAR MECHANISM OF COSMOLOGICAL RECOMBINATION

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According to the standard mechanism of recombination two charged particles an electron, and a proton participated in the formation of atomic hydrogen. An electron and a proton combined efficiently into the hydrogen atom only in a highly excited state, from which a rapid cascade occurred into a state with the principal quantum number  $n = 2$ .

In our study, we assume that an electron collides with two protons situated one far from another, emits a photon, and creates a quasi-molecule,  $H_2^+$  in a highly excited state [1]. If  $H_2^+$  is formed in a repulsive state, it rapidly dissociates into a proton and the excited hydrogen atom, which then cascades downward. This mechanism is analogous to the standard mechanism of recombination. However, if  $H_2^+$  is formed in an attractive state, the protons involved in recombination approach each other, and the quasi-molecule descends into a low-lying state which might be repulsive or attractive (see Fig.1 in [2]). The quasi-molecular mechanism of recombination (QMR) thus produces  $H$  as well as  $H_2^+$  in the ground state.

Obviously, the QMR was significant at the pre-recombination stage of the evolution of the Universe (redshift  $z > 2000$ ) when the temperature and density of matter were higher than subsequently. The estimation shows that at that period the average distance between protons in the primordial plasma was about  $10^6 a_0$ , where  $a_0$  is the radius of the first Bohr orbital in the hydrogen atom.

The purpose of the present study is to answer the question could the nearest neighboring proton impact cosmological recombination at such distances  $R$  between protons? For this, a scheme of calculation based on the QMR was elaborated and applied to the calculation of probabilities of free-bound transitions into a highly excited attractive state of  $H_2^+$ . For large  $R$  the transition probability is expressible as

$$W_{i \rightarrow f}(R) = W_{i \rightarrow f}^{(0)} + \frac{1}{R} W_{i \rightarrow f}^{(1)} + O(R^{-2}), \quad (1)$$

in which  $W_{i,f}^{(0)}$  determines the transition probability on an isolated proton, and  $W_{i,f}^{(1)}$  accounts for a correction caused by the participation of another proton in recombination. Calculations revealed that compared with the first term the contribution of the second term in (1) increases from 0.001 at  $n=100$  to 0.05 at  $n=400$ . This means that for highly excited states the impact of the QMR on cosmological recombination was perceptible.

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## AN ATOMIC DATA OPTIMIZATION METHOD FOR IMPROVED KILONOVA OPACITY MODELING

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In 2017, the identification of an electromagnetic counterpart to the gravitational wave signal GW170817 constituted direct evidence for the production of r-process elements during the collision of neutron stars [1]. One of the principal sources of uncertainty for modeling the resulting kilonova, essential to probe and characterize the ejecta, comes from the atomic data used. Small relative errors (e.g. few percent) in the transition wavelengths, or larger errors in the oscillation strengths (tens of percent), can make interpretation of the spectra or the identification of features of specific elements [2,3] difficult or even impossible to achieve. The high degree of complexity of open f-shell elements, expected to be present in the ejecta, in combination with the necessity for large datasets to comprehensively capture opacity behavior across both the optical and infrared ranges, makes the use of full *ab initio* codes impractical in most instances due to their intensive computational demands [4]

Using the publicly available Flexible Atomic Code software package [5], we have developed an optimization procedure to provide atomic data (energy levels and oscillator strengths) which attempts to improve consistency with available experimental or *ab initio* data while retaining efficiency in the calculations. In this work we analyze the sensitivity of the data to the optimization method and how it allows for a controlled and systematic improvement of accuracy when compared to other methods [6,7]. Furthermore we investigate how this optimization technique affects our calculations as well its impact on line-by-line and gray opacity data.

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## Exploring ab-initio and semi-empirical small-scale atomic structure models of neutron-capture elements

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Recent advancements in astrophysics, such as the James Webb space telescope (JWST) and the LIGO/Virgo gravitational wave detectors, have introduced new demands on atomic physics. With the JWST operating in the infrared spectral regime, and the LIGO/Virgo leading to the ground-breaking discovery of the first neutron-star-merger event accompanied by a kilonova transient (arguably a dominant production site for neutron capture elements) [1], have highlighted the need for reliable atomic data for the heavier elements, in particular in the infrared.

However, the current databases are both incomplete and poor in quality when it comes to heavy elements. This lack of information on atomic energy levels and processes is partly due to the complexities involved in carrying out atomic structure calculations for many of these elements, notably the lanthanides.

A significant challenge posed by lanthanides is the presence of multiple configurations with many levels and overlapping energies, giving rise to perturbing states. These elements often have orbitals that are closely aligned energetically so that different occupations lead to configurations of similar energies. Current state-of-the-art atomic structure codes assume an orthonormal orbital basis set. However, separate calculations of two competing configurations reveal significant non-orthonormalities between the orbitals of each configuration. This can lead to inaccurate expectation values if not taken into account properly.

In this contribution, we present methods for performing atomic structure calculations that address this critical issue while also ensuring that the wavefunctions remain compact enough for efficient computations of collisional-radiative properties across a wide range of atomic systems needed, for instance, in kilonova spectral modeling. Taking neutral gold as a representative system and using the relativistic atomic structure code GRASP2018 [2], we explore targeted optimization techniques to treat the orbital non-orthonormalities. Moreover, we investigate semi-empirical rescalings of diagonal matrix elements to further improve the quality of the wavefunction, as recently discussed in the context of the GRASP code by Li et al. [3].

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## A VARIATIONAL ATOMIC MODEL OF PLASMA ACCOUNTING FOR ION RADIAL CORRELATIONS AND ELECTRONIC STRUCTURE OF IONS

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We report on a new model of ion-electron plasma (or nucleus-electron plasma) that accounts for the electronic structure around nuclei (i.e. ion structure) as well as for ion-ion correlations [1]. The model equations are obtained through the minimization of an approximate free-energy functional, and it is shown that the model fulfills the virial theorem.

The main hypotheses of this model are 1) nuclei are treated as classical indistinguishable particles 2) electronic density is seen as a superposition of a uniform background and spherically-symmetric distributions around each nucleus (system of ions in a plasma) 3) free energy is approached using a cluster expansion 4) resulting ion fluid is modeled through an approximate integral equation.

In this poster we describe the set of hypotheses of this model, sketch the derivation of the model equations and comment on them. We show how this model fulfills the virial theorem, allowing a sound definition of the related thermodynamic quantities. Then, we show some preliminary numerical results regarding the equation of state, as well as quantities related to radiative properties, such as the oscillator strengths. These results are compared with results from other models such as VAAQP or INFERNO. Finally we discuss some limitations of the model.

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## STELLAR OPACITIES IN LAB USING A HIGH INTENSITY LASER

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The opacity of the Sun radiative zone is a key to understanding energy flux in the Sun interior as well as its structure. The opacity of the radiative zone is mostly governed by oxygen, iron and neon absorption [1], but most of the questioning lies on the iron opacity.

In 2015, experiments carried out on the Z-machine exhibited large discrepancies between experimental results and modeling [2]. Ever since, only a handful of experiments challenge to create in laboratory solar-relevant conditions. In this poster, I will present the results obtained on a new opacity platform at LULI laboratory, based on isochoric heating of iron by an ultra-intense laser. These results will be compared to state-of-the-art atomic simulations.

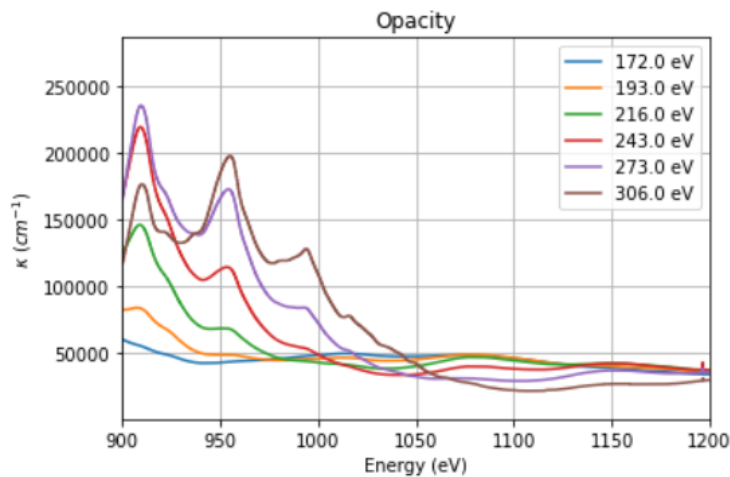


Figure 1: Simulated opacity of the heated iron at different temperature using OP.

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## Erbium Optical Spectra from Pellet Ablation Cloud in the Large Helical Device for Laboratory Assessment of Atomic Data

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The atomic data of heavy elements, especially rare-earth metals, plays a crucial role in enhancing our understanding and interpreting the kilonova spectra and the underlying astrophysical processes. Among these elements, Erbium (Er) is particularly intriguing to look for in kilonova spectra [1]. In order to assess the atomic data emission spectra from Er are measured in the optical region. In the present experiment, Er was injected into the core plasma of the Large Helical Device (LHD) through carbon pellets containing Er powders. As soon as the pellet entered in the plasma, the intense heat flux generated by the plasma caused immediate ablation on its surface, forming an ablation cloud temporarily in its vicinity. The radiation spectra from this ablation cloud were measured in the 380- 400 nm region. Most of the observed lines in the spectra belonged to CII and ErII ions. To analyze the observed emission line spectra, a line shape analysis incorporating Doppler and Stark broadening was employed. As the current plasma is in a magnetic field (~2.75T), a contribution to line broadening due to several Zeeman components was also considered. From the stark width, the electron density of the plasma was evaluated. Since the electron density of the ablation cloud was high, we could assume local thermal equilibrium (LTE) for the ablation cloud plasma. Additionally, the transition probability of the Er II line observed at 393.863 nm was obtained through Boltzmann plot analysis [2].

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## STUDY OF B-LIKE IONS X-RAY EMISSION SPECTRA IN AN ELECTRON-CYCLOTRON RESONANCE ION SOURCE PLASMA

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Chandra and XMM-Newton brought astrophysical x-ray spectroscopy to a new era by providing the first high-resolution (0.5% in the X-ray band) measurements. These improvements have led to a need for more precise atomic data to interpret the astrophysical measurements. Later measurements, showing unknown x-ray contributions, drew the question of new physics [1], which was finally resolved by new measurements using ion sources [2]. The extensive usage of microcalorimeters in recent (Hitomi) and future (Athena/XFU and XRISM) missions give new perspectives for x-ray measurements of astrophysical objects [3]. Concurrently, thanks to modern intense ion sources [4], in-lab precise measurements of transitions in highly-charged ions, like in sulfur, allow to improve the modelling of the measurements [5]. We present here new reference-free high-precision measurements of x-ray transitions in boron-like argon and sulfur. The measurements were performed with an Electron Cyclotron Resonance Ion Source and a double-crystal spectrometer installed in Paris at Sorbonne Université [6]. These spectra show multiple transitions, which required the use of Bayesian model selection methods to determine the number of spectral components and their characteristic profile. This is performed using the nested sampling method implemented in the nested fit code [7] which will be also introduced.

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## TRANSITION PROBABILITY MEASUREMENTS FOR LANTHANIDE ELEMENTS USING LASER-INDUCED BREAKDOWN SPECTROSCOPY

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Atomic data of rare-earth elements are having great importance in many fields, especially in astrophysics. Recently, the study of kilonovae emissions led scientists to consider neutron star mergers as a source of heavy elements, such as lanthanides. Thus, the necessity of highly accurate and precise spectroscopic data, especially the transition probability, increased drastically for the radiative transfer simulation of kilonovae [1]. In this poster, we present transition probability measurements for some lanthanide elements using laser-induced breakdown spectroscopy (LIBS).

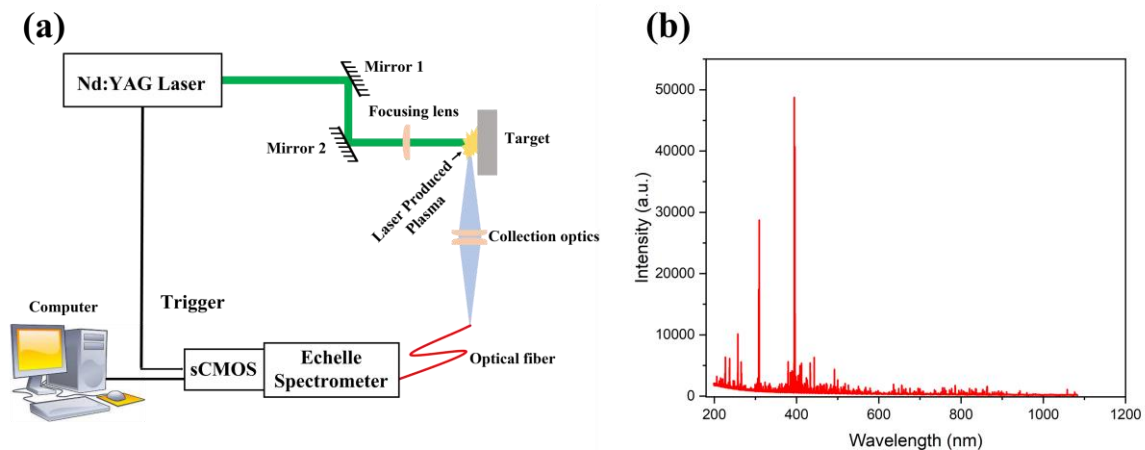


Figure 1: (a) Schematic of the experimental setup. (b) LIBS spectrum of an Al-La alloy.

LIBS is an atomic emission spectroscopic technique generally used for elemental analysis [2]. Figure 1(a) shows a schematic diagram of the LIBS setup. For evaluating the transition probabilities, an alloy of aluminum containing 5% lanthanoid elements (La, Ce, and Er) is used as a target placed in a chamber filled with Ar gas ( $\sim 200$  Pa). A typical LIBS spectrum of Al-La alloy is shown in figure 1(b). Considering the LTE condition of the plasma, the Boltzmann plot method is used for deducing the transition probabilities of emission lines which are not reported in the NIST atomic spectra database [3].

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## HIGH-RESOLUTION TALIF SPECTROSCOPY FOR OPTICAL DIAGNOSTICS IN COLD PLASMAS

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Two-photon absorption laser induced fluorescence (TALIF) method is commonly used to measure atomic densities and temperatures in gaseous media, especially for plasma diagnostics. TALIF consists in recording the fluorescence following the two-photon excitation of an atomic species. For oxygen density measurements, a widespread protocol is to compare the fluorescence yield to that measured in Xe vapor, the density of which can be known straightforwardly, when illuminated by the same optical system. However, quantitative analysis relies on knowledge of the ratio of both two-photon cross-sections  $\sigma^{(2)}$  involved. Direct measurement of the integrated cross-section  $\sigma^{(2)}(\text{Xe})$  can be done by non-linear absorption spectroscopy [1]. We determined the integrated cross-section for the  $6p'[3/2]_2$  level, and find a value that is more than a factor of 2 smaller than the admitted one.

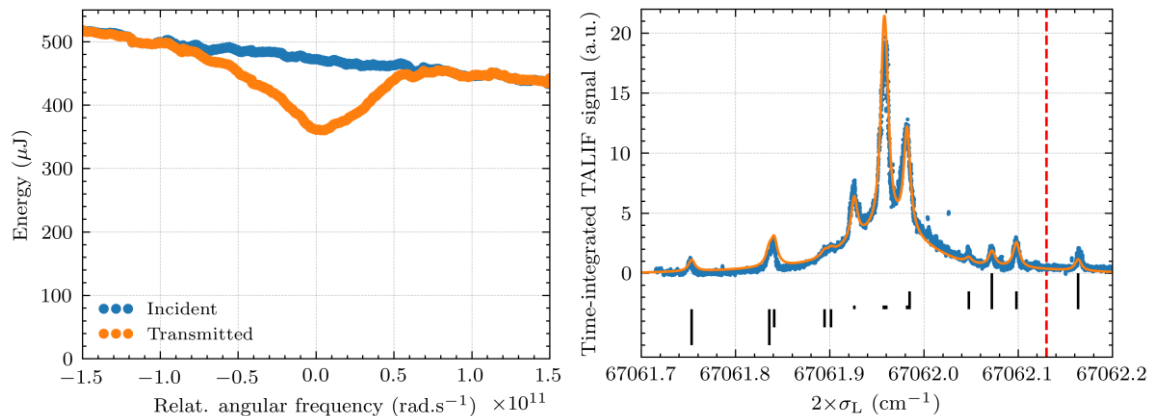


Figure 1: Left: Two-photon absorption spectra of the  $6p'[3/2]_2$  resonance of Xe. ( $n = 1.63 \times 10^{24}$   $\text{at}\cdot\text{m}^{-3}$ ,  $L = 51$  cm,  $w_x \sim w_y \sim 310$   $\mu\text{m}$  and pulse duration of 6.4 ns). Right: Doppler-free fluorescence spectra, following excitation of the ( $^3\text{P}_2$ )  $6p^2[1]_0^o_{3/2}$  of I.

TALIF spectroscopy also leads to the determination of the temperature of atomic species in the plasma, via Doppler broadening, provided that a sufficiently narrow-line laser is used. For this purpose, we have specially built [2] a pulsed single-mode ns-laser. Furthermore, for atoms with a non-zero nuclear spin, hyperfine structures can underlie the Doppler profile. These structures have been determined for iodine and xenon by Doppler-free spectroscopy [3,4]. For noble gases, we have established a relation that makes a rough estimation of the hyperfine structure possible as a function of atomic quantum numbers [4].

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## **Development and Commissioning of the UNIST Electron Beam Ion Trap for X-Ray Spectroscopy of the Highly Charged Ions at PAL-XFEL**

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An electron beam ion trap (EBIT) is a device that creates and studies highly charged ions (HCIs). To maximize its portability to move in and away from the accelerator beamlines, we adopt permanent magnets to reduce the size and maintenance cost. A 0.84 T magnetic field at the trap center gives a trap capacity of  $10^7$ . By sweeping the electron beam energy from 2.4 to 3.3 keV at 10 mA, the silicon drift detector successfully measures KLL lines of the highly charged states of argon and confirms the existence of up to He-like argon. Before the highly charged iron measurement for astrophysics purposes, we conducted preliminary experiments on connecting the EBIT with the PAL-XFEL (Pohang Accelerator Laboratory X-ray Free Electron Laser) hard X-ray beamline over two R&D beam times. We report our first operation at the XFEL facility, demonstrating the x-ray fluorescence measurement using the highly charged argon.

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## EXPERIMENTAL METASTABLE LIFETIMES AT DESIREE STORAGE RING – FIRST STOP : BARIUM

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We are developing a laser probing technique at the Double Electrostatic Cryogenic Storage Ring DESIREE at Stockholm university, Sweden [1]. The excellent vacuum and temperature conditions allows to store the barium ions  $\text{Ba}^+$  with a beam lifetime of 500s. We present our first measurements of the  $5d\ ^2D_{3/2}$  metastable state of Ba II with a lifetime around 80 s with a 1% uncertainty.

We apply a pump and probe technique utilizing two lasers. One red laser emptying the metastable state and probing the population, and a blue laser repopulating the state by transferring all the population from the ground state  $6s\ ^2S_{1/2}$  to the  $5d\ ^2D_{3/2}$  state investigated. By varying the time delay between pump and probe, the lifetime curve is built up.

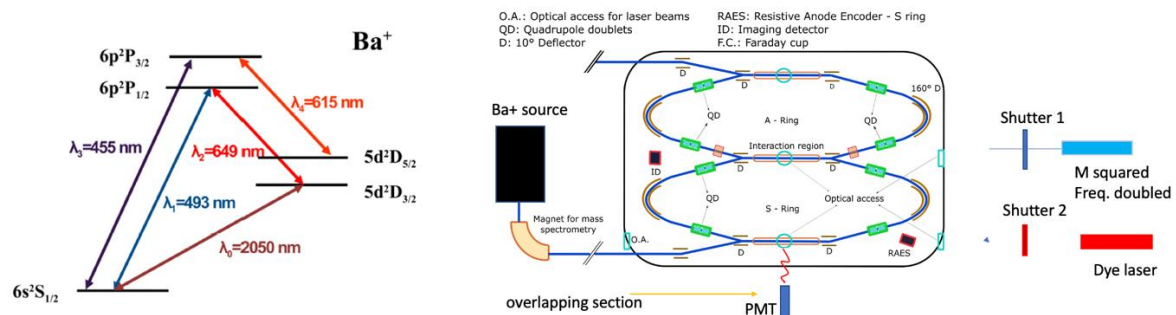


Figure 1: *left*: Energy level diagram of Ba II, with metastable  $5d\ ^2D_{3/2}$ . *Right*: The DESIREE storage ring and the experimental setup

Thanks to the excellent storage conditions, we see only very small systematic effects such as repopulation and collisional quenching. Future studies will include more complex spectra such as Fe II.

A consortium consisting of Stockholm University (SU), the University of Gothenburg (UGOT) and Malmö University (MaU) operate DESIREE as a national infrastructure since January 2018 with support from the Swedish research Council VR. Authors from UL were supported by ERDF project No. 1.1.1.5/19/A/003: and ERDF project No. 1.1.1.1/19/A/144.

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# ATOMIC DATA AND OPACITY CALCULATIONS IN MODERATELY CHARGED LANTHANIDE IONS IN THE CONTEXT OF KILONOVA EMISSION MODELING

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The LIGO-VIRGO collaboration observed a neutron star merger (GW170817 event) thanks to the first detection of gravitational waves. They also detected the electromagnetic emission of the gigantic explosion called kilonova which is a hot and radioactive matter ejected in the space [1]. In the latter, nuclear reactions take place and form heavy nuclei such as lanthanides ( $Z = 57 - 71$ ) which contribute strongly to the luminosity and spectra of the kilonova. Such elements produce millions of lines due to their complex configurations characterized by an unfilled 4f subshell [2].

To interpret the spectrum of a kilonova, it is therefore crucial to precisely know the radiative parameters characterizing these elements. In recent years, several studies have been carried out (e.g. [3-4]), for the first degrees of ionisation (up to 3+) but almost all these investigations were limited to the analysis of kilonovae in a temperature range below 20000 K. In order to extend the study to early phases of kilonovae (i.e.  $T > 20000$  K), it is essential to know the radiative parameters of lanthanide ions in higher charge stages (see e.g. [5-8]).

The present work focusses on atomic data and opacity calculations for lanthanides from the fourth to the ninth degree of ionization, for typical ejecta conditions such as the density  $\rho = 10^{-10}$  g cm<sup>-3</sup>, the time after the merger  $t = 0.1$  day and temperatures  $T > 20000$  K. In order to do that, we used the pseudo-relativistic Hartree-Fock (HFR) method as implemented in Cowan's codes [9] to calculate the radiative parameters. The expansion formalism [10-12] was then used in order to compute the opacity, at 25000 K, 35000 K and 40000 K, which are extremely important for astrophysicists [13].

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# ATOMIC DATA AND OPACITY CALCULATIONS IN Nb, Ag, Hf, Os AND Au IONS FOR KILONOVA SPECTRAL ANALYSES

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Neutron star (NS) mergers are at the origin of gravitational waves (GW) detected by LIGO/Virgo interferometers [1]. Such events produce a large amount of elements heavier than iron by a rapid neutron capture (r-process) nucleosynthesis. Among these elements, those belonging to the fifth and sixth rows of the periodic table, are the greatest contributors to the opacity affecting the kilonova spectra, after the lanthanides and actinides. In the present work, new calculations of atomic structures and radiative parameters (wavelengths and oscillator strengths) are reported for a large number of spectral lines in some representative elements belonging to the fifth row, namely Nb ( $Z = 41$ ) and Ag ( $Z = 47$ ), and belonging to the sixth row, namely Hf ( $Z = 72$ ), Os ( $Z = 76$ ) and Au ( $Z = 79$ ) from neutral to triply ionized states. The results obtained were used to calculate the expansion opacities characterizing the kilonova signal observed resulting from the collision of two NS, for typical conditions corresponding to time after the merger  $t = 1$  day, the temperature in the ejecta  $T \leq 15000$  K, and a density of  $\rho = 10^{-13}$  g.cm<sup>-3</sup> [2]. The results presented in this work are the most complete currently available and are useful for astrophysicists to interpret kilonova spectra.

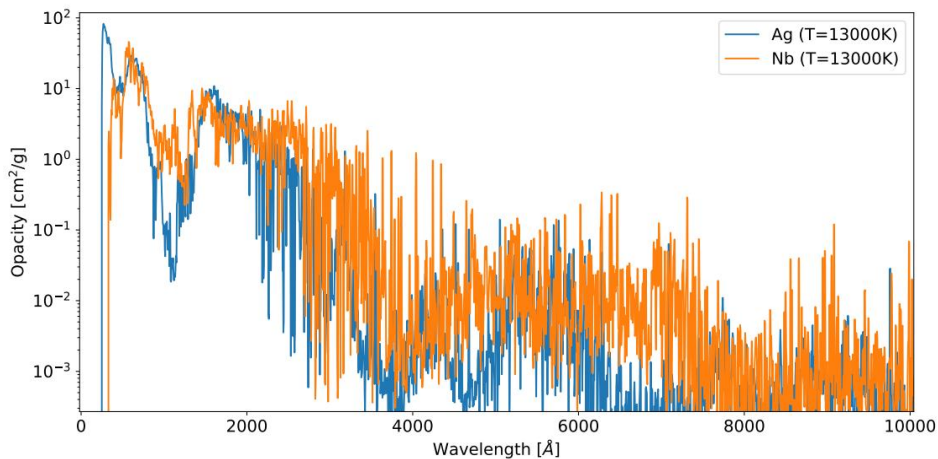


Figure 1: Expansion opacity for Nb and Ag, calculated with  $T = 13\,000$  K, with  $\rho = 10^{-13}$  g.cm<sup>-3</sup>,  $t = 1$  d and  $\Delta\lambda = 10$  Å.

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## Atomic calculations for V – XI ionized *r*-process elements for early kilonova

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We perform the atomic structure calculations by using Hebrew University Lawrence Livermore Atomic Code or HULLAC [1] to construct the data for the energy levels and transition probabilities for all *r*-process elements from Ca - Ra ( $Z = 20-88$ ) ionized to the states V – XI [2, 3, 5]. Using the atomic data, we calculate the bound-bound opacities for the elements ionized to different states (see Fig. 1 for variation of mean opacities for different ionization at density  $10^{-10}$  g cm<sup>-3</sup>). Such opacities are suitable to calculate the light curves at an early time ( $t < 1$  day) of the astronomical transient kilonova from neutron star merger. Understanding the light curves of kilonova from early time provides the hint to understand the origin of heavy *r*-process elements and hence, is of extreme importance.

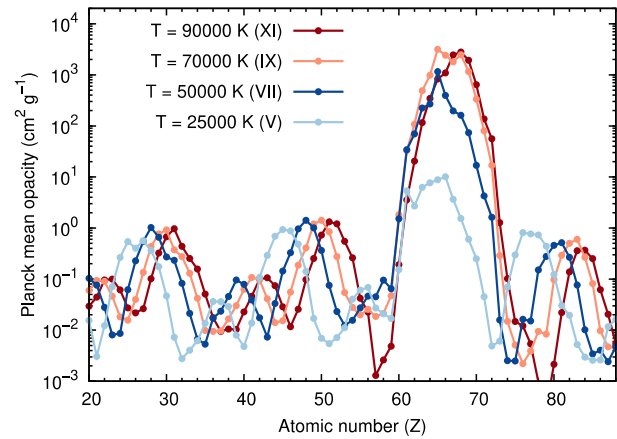


Figure 1: The mean opacities for different elements suitable to calculate early kilonova ( $t < 1$  day) from the binary neutron star merger (Banerjee et al, 2023, submitted to ApJ).

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## **DETAILED NLTE ABUNDANCE ANALYSIS OF 20 NUCLEAR STELLAR CLUSTER/DISK STARS**

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Nuclear star clusters are near ubiquitous in galaxies: they are present in ~70% of early- and late-type galaxies with stellar masses above  $10^8$ - $10^{10}$  solar masses. Further, the masses of nuclear star clusters show scaling relationships with the masses of their host galaxies, which suggests the idea that the nuclei of galaxies may have co-evolved with their hosts. Also supported by simulations, the very inner parts of galaxies are thought to provide clues to processes that shape galaxy formation and evolution.

We present a detailed NLTE abundance analysis of 20 stars in the Nuclear Star Cluster and the Nuclear Stellar Disk using recently calculated NLTE departure coefficients. We compare the results with an equivalent analysis of stars located in the disk further out in the Galaxy. Like previously analysed and published silicon abundances for the same set of stars, we show that even for elements such as calcium there is a significant difference between stars located in the Nuclear Stellar Cluster/Disk and stars located further out in the Milky Way disk.

# TRANSITION DATA FOR NEUTRAL CARBON RYDBERG LEVELS BENCHMARKED AGAINST SOLAR UV OBSERVATIONS

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A wealth of lines from Rydberg levels in neutral carbon are present in astrophysical spectra, from stellar atmospheres to the interstellar medium. In solar ultraviolet (UV) spectra, the lines are emitted in the lower atmosphere, the chromosphere, which is a poorly understood region with fewer diagnostics. Lines are observed routinely from these levels, up to  $n=24$  [1], and the transition data are important also in modelling UV lines emitted from lower levels.

The frozen cores approximation using R-Matrix codes was shown to be successful in calculating data for Rydberg levels in neutral carbon [2]. The calculation, however, included levels only up to  $n=10$  and decays to the  $2s^2 2p^2 \ ^3P$  term. The present work uses the same approximation to calculate transition data up to  $n=30$  and for decays to the three terms in the ground configuration, all of which are present in solar spectra. Wavelengths are typically within  $10\text{m}\text{\AA}$  of experimental values and transition rates within 2% of other theoretical data.

Levels above  $n=11$  should be in local thermodynamic equilibrium at solar densities, which allows a synthetic spectrum to be calculated to further assess the new data. It shows excellent agreement with high resolution spectroscopy of the solar atmosphere [3] in both wavelengths and relative intensities of the lines. More than 20 new line identifications are found, mainly in the  $1445\text{-}1500\text{\AA}$  wavelength range. Optical depth effects are also shown to be present in the observations.

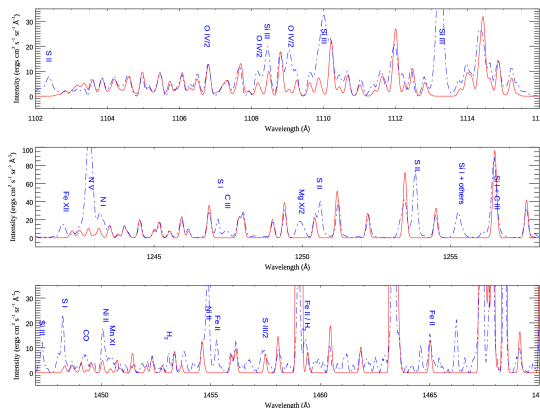


Figure 1: Comparison of synthetic spectrum with solar observations: red line – synthetic spectrum, blue dashed – solar observations. Known lines from other ions are highlighted.

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## Japan-Lithuania Opacity Database for Kilonova

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We have recently constructed optical absorption data of r-process element ions [1], which are in high demand for the analysis of kilonova observation associated with neutron star mergers. The data were developed by theoretical calculations using HULLAC code [2], and made a database available at NIFS [3] in cooperation of Japan and Lithuanian experts. The database contains energy level and oscillator strength data of neutral through triply charged ions for most of the r-process elements ( $Z = 26 - 88$ ). In the database, bound-bound Plank mean opacities calculated with those atomic data for abundance distributions at given electron fractions ( $Ye$ ) are also available at temperature and density grids for 1,000 – 25,500 K and  $10^{-19.5} - 10^{-5} \text{ g/cm}^3$ , respectively.

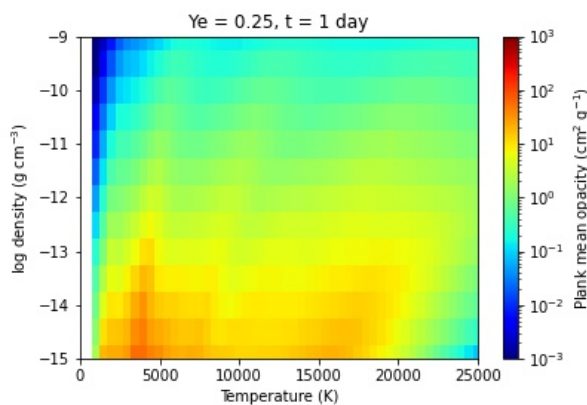


Fig 1. Plank mean opacity for  $Ye = 0.25$  and 1 day after the merger.

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# Zeeman Spectroscopy of Tellurium

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Tellurium spectroscopic studies have received a lot of interest recently as a result of the use of Te-like systems in highly accurate optical clocks [1]. However, Te's complicated multielectron spectra, which contain several  $p^k n^l$  electronic configurations, present a challenge for both theoretical and experimental spectroscopic studies. The last experimental work on the structure of Te I was published in 1982-1983. Previous theoretical work on Te are mostly limited to ground and low excited states. Therefore, in this work, Zeeman structure of eight lines of  $^{130}\text{Te}$  are studied using high-resolution emission spectroscopy in the range 640-990 nm (see Figure 1). Landé  $g_J$  factors for seven levels were determined for the first time. The validity of present experimental data is proved by performing theoretical calculations using the multiconfiguration Dirac-Hatree-Fock (MCDHF) method incorporated in GRASP2018 [2] package. The calculations were performed for 53 levels belonging to the  $5p^4$ ,  $5p^3 6s$ ,  $5p^3 5d$ ,  $5p^3 6p$ ,  $5p^3 8s$ ,  $5p^3 8d$  and  $5p^3 9d$  configurations. Moreover, theoretical Landé  $g_J$  factors of 19 levels are new, and no experimental values are available for comparison.

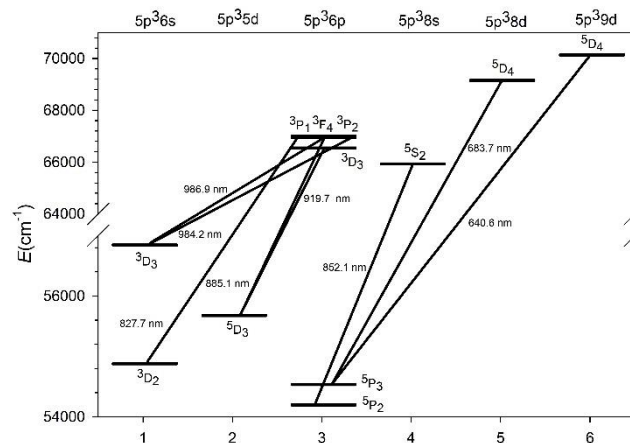


Figure 1: Energy-level diagram of Te I with investigated transitions.

The average level of agreement between the current theoretical and experimental findings is 2.4%, with individual data pair levels ranging from 0.6% to 4.8. The percentage average discrepancy between the theoretical energy predicted in this work and the NIST values is only 1.4%. The agreement between the calculated and NIST values of the Landé factors is, on average less than 2.5 %. We believe the present studies extends the existing data on Landé factors.

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## SIMULATION OF Pm-LIKE BISMUTH SPECTRA IN AN EBIT

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We use a multiconfiguration Dirac-Fock code [1,2] to calculate electronic excitation cross sections and radiative decay transition probabilities for a large number of atomic levels in Pm-like bismuth. By numerically solving a set of equilibrium equations we were able to obtain the level populations of the  $4f^{14}5s$ ,  $4f^{13}5s5f$ ,  $4f^{13}5s5d$ ,  $4f^{13}5s5p$ , and  $4f^{13}5s^2$  configurations and synthesized spectra for a number of electronic density values in an EBIT for 640 keV incident electron energy.

The synthesized spectrum we obtained for  $10^{10} \text{ cm}^{-3}$  electronic density agrees qualitatively with the experimental data of Kobayashi et al. [3]. We found significant differences between our simulations and Kobayashi's for several electronic density values.

The emission lines position and relative intensity can also be compared with laser produced plasma spectra, to improve the identification of the Pm-like ions and provide experimental values of electron density at those plasma conditions.

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# Measurement of Charge Exchange Cross Sections for Highly Charged Ions Collision with He

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The charge exchange (CX) process between ions and the neutral target is of great significance in explaining the X-ray emission spectrum of the solar system. To investigate the CX process in the lab, an experimental instrument setup based on the 150 kV high-voltage platform with an electron cyclotron resonance (ECR) ion source at Fudan University was built to measure the absolute single- and double-electron capture cross sections and  $nl$ -resolved state-selective charge exchange cross sections between low-energy highly charged ions and neutral targets. The  $nl$  state-selective charge exchange cross-section of  $\text{Ar}^{8+}$  colliding with He, and the absolute and state-selective cross sections between  $\text{O}^{6+}$  and He were obtained [1-2].

As shown in Fig. 1, a series of measurements on the charge exchange of  $\text{Ar}^{8+}$  ion with He were performed in the collision energy range from 1.4 to 20 keV/u. It was found electrons were mainly captured in the  $n = 4$  state of  $\text{Ar}^{7+}$  ions compared to the  $n = 3, 5,$  and  $6$  captures, which was in agreement with the scaling law prediction for dominant capture. And the relative cross sections were also reported for  $4s-$ ,  $4p-$ ,  $4d-$ , and  $4f$ -resolved state-selective capture [1].

To further extend the research, the investigation of the singlet charge exchange process of  $\text{O}^{6+}$  and He was performed both experimentally and theoretically. The total and state-selective ( $n = 3, 4, 5$  and partially  $3s$ ) cross sections for the singlet electron capture have been measured in the energy range of 2.63-37.5 keV/u. The state-selective cross section of  $n = 5$  above 4.5 keV/u was reported experimentally for the first time. Total and state-selective cross sections were also calculated in the energy range of 0.3-100 keV/u, performing a good agreement with the experiment result. And the importance of electronic correlation was found compared with the previous methods [2].

Furthermore, the total electron-capture cross section between  $\text{O}^{6+}$  with  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{H}_2$ , and  $\text{N}_2$  has been measured [3].

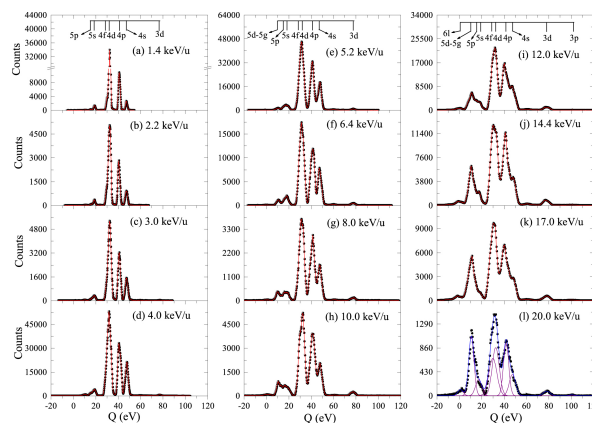


Figure 1: The measured Q spectra of CX between  $\text{Ar}^{8+}$  and He.

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# The role of the $3 \rightarrow 5$ excitation channels in the dielectronic recombination of M-shell Fe ions: the Na and Mg isoelectronic sequences

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The important role played by dielectronic recombination (DR) of M-shell Fe ions in the observed absorption X-ray spectra of Seyfert galaxies [1,2] have encouraged a thorough investigation of the related plasma DR rate coefficients in support of astrophysical observations. So far, theoretical modeling of such processes has accounted for the sole contributions due to  $\Delta n = 0,1$  excitation channels (see, for instance, [1]). However, it was pointed out that at reasonably high temperatures even the neglected  $\Delta n = 2$  channels may remarkably contribute to the total temperature-dependent DR rates [3]. This has spurred us to investigating the contribution of the  $\Delta n = 2$  excitation channels for the  $3 \rightarrow 5$  electron excitations to the plasma rate coefficients of initially Na-like and Mg-like Fe ions in the  $10^5 - 10^9$  K temperature range, by means of the Multi-Configurational Dirac-Hartree-Fock method. As a result, the contribution to the total plasma DR rates due to this excitation channel was found to be relevant and comparable to the  $\Delta n = 0,1$  analogs.

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