

# Oral Contributions



# TRANSITION INTENSITIES OF TRIVALENT LANTHANIDE IONS IN SOLIDS: EXTENSION OF JUDD-OFELT THEORY ON $\text{Eu}^{3+}$ , $\text{Nd}^{3+}$ AND $\text{Er}^{3+}$

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Lanthanides are widely used in the industry. For example, they are used as the active ions in luminescent materials used in optoelectronics applications, most notably the Nd:YAG laser. Erbium-doped fiber amplifiers are significant devices in optical-fiber communication systems. These and other applications are based on optical transitions between levels of the ground configuration of the trivalent lanthanide ions. Being forbidden in the electric-dipole approximation, those transitions are activated by the crystal-field potential created by the host material. The Judd-Ofelt (JO) theory has been successfully applied since 60 years, to interpret the intensities of absorption and emissions lines of crystals and glasses doped with trivalent lanthanide ions. Despite the fact that it is remarkably efficient for many cases, the standard version of the JO theory cannot reproduce some of the observed transitions, because of its strong selection rules [1-2].

In order to overcome this issue we present a modified version of the JO theory, where the properties of the dopant are calculated with well-established atomic-structure techniques, while the influence of the crystal-field potential is described as a perturbation, by three adjustable parameters [3]. In the extension we introduce also the wavelength-dependence of the refractive index of the host material with the help of the Sellmeier equation. We test the validity of our model on three ions:  $\text{Eu}^{3+}$ ,  $\text{Nd}^{3+}$  and  $\text{Er}^{3+}$ . The results of the extension are very good (see figure 1). We are able to give a physical insight into all the transitions within the ground electronic configuration, and also to reproduce quantitatively experimental absorption oscillator strengths.

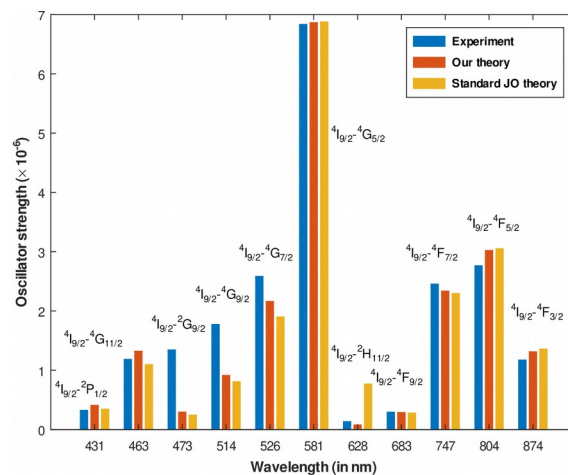


Figure 1: Comparison between experimental [4] and theoretical oscillator strengths of absorption, plotted as function of the transition wavelength (not at scale) for  $\text{Nd}^{3+}$ .

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## High resolution vacuum ultraviolet absorption spectroscopy: determination of reactive species' oscillator strengths

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DESIRS is a VUV (Vacuum UltraViolet) beamline at the synchrotron SOLEIL facility characterized by high flux, high resolution, spectral purity, and variable polarization. DESIRS is equipped with several state-of-the-art instruments, including an i2PEPICO set-up and an ion trap, for the study of VUV photon-induced processes on isolated gas phase samples, such as cold molecules, radicals, (chiral) biomolecules, large ionic biopolymers, clusters and nanoparticles[1]. In addition, the VUV-FTS (VUV-Fourier Transform Spectrometry) experimental branch has been designed to provide both high spectral resolution and broad band capability[2,3]. In operation since 2008, this permanent endstation has permitted the study of small molecules, revisiting the spectroscopy of fundamental stable molecules such as CO, N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub> or H<sub>2</sub>O presenting an evident astrophysical interest. Recently, various set-ups aiming at the production of transient species such as radicals have been developed and led to an increased knowledge including band oscillator strengths on key radical species such as OH, S<sub>2</sub>, CH<sub>3</sub> and SO, VUV spectroscopic studies of atomic species [4,5], or application to plasma modelization[6]. An overview of the most significant achievements will be shown, with a highlight on the OH radical[7].

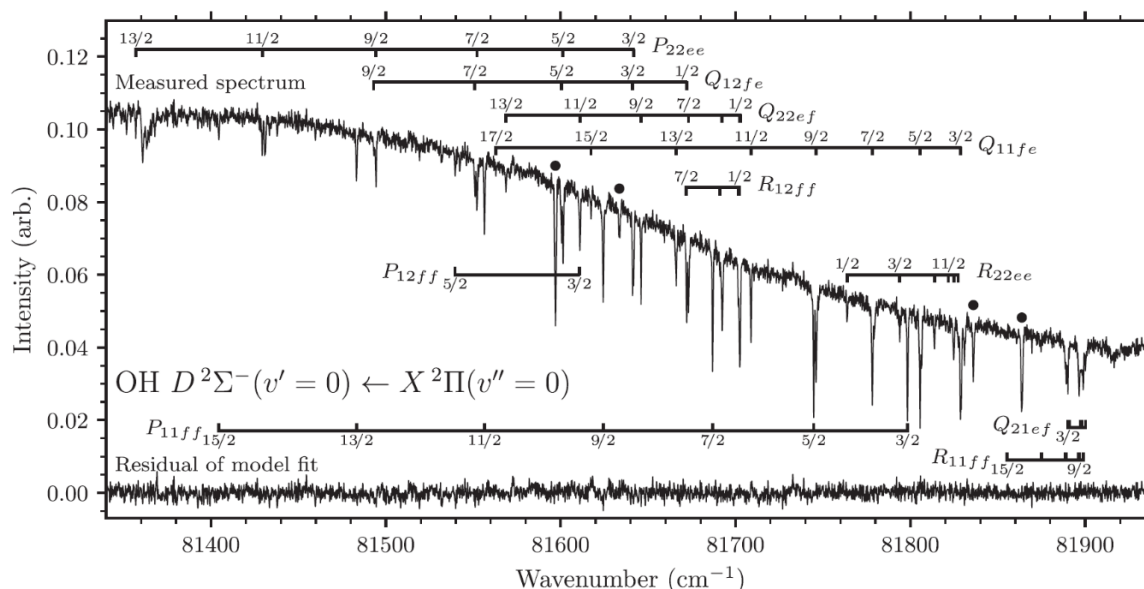


Figure 1: Assigned experimental spectrum showing the OH  $D^2\Sigma^-(v' = 0) \leftarrow X^2\Pi(v'' = 0)$  absorption band (RF discharge, FTS spectral resolution:  $0.27 \text{ cm}^{-1}$ ).

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## HYPERFINE INTERACTION AFFECTING THE CHARGE-STATE DISTRIBUTION OF HIGHLY CHARGED ION PLASMA

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In a recent electron beam ion trap (EBIT) experiment we have found that the charge state distribution of highly charged ions can be strongly affected by metastable energy levels that accumulate considerable population [1]. In an EBIT, where the ion cloud in its equilibrium generally consists of a narrow distribution of charge states, the effect strongly depends on the density of the electrons. Ultimately the population distribution among levels of the different ions, together with the transition rates from these levels determine the emitted spectra of plasmas. As a result, these spectra can serve as sensitive diagnostic tools for environments where metastable ions are present.

In a series of measurements, we used the EBIT of the National Institute of Standards and Technology (NIST) to confine and probe Pr and Nd lanthanide ions at different electron beam energies and densities [1-3]. Spectra were recorded by a recently installed transition edge (TES) sensor x-ray microcalorimeter with good energy and photon arrival time resolution [4]. The non-Maxwellian plasma was modeled by collisional-radiative calculations [5] to reliably predict the spectral emission of the ion cloud [1-3]. Our analysis showed that the finely tuned charge state distribution near the Ni-like charge state is strongly affected by the metastable population fraction at  $10^{10}$ - $10^{12}$  cm<sup>-3</sup> densities. The time evolution and the equilibrium intensity ratio of spectral lines showed that isotope-dependent hyperfine interaction strongly influences the population dynamics in these systems.

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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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## 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  $Ba^+$  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.

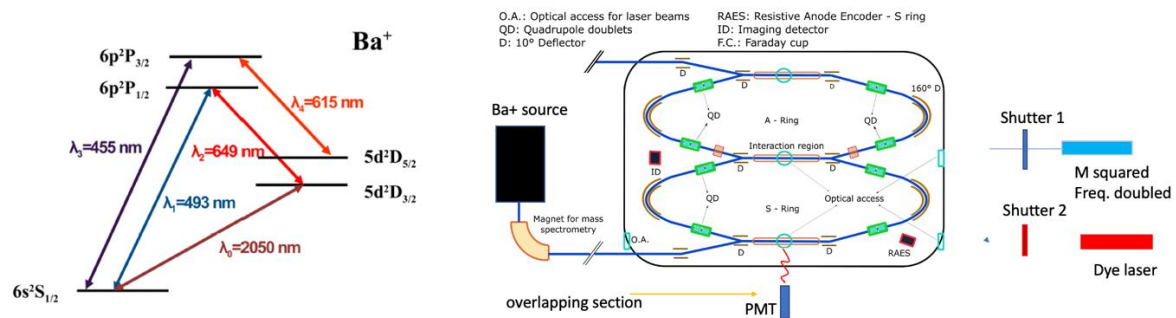


Figure 1: *left*: Energy level diagram of Ba II, with metastable  $5d\ ^2D_{3/2}$ . *Right*: The DESIREE storage ring and the experimental setup

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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## GRASP and COMPAS for ASOS

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There is a well-established interest in the General(-purpose) Relativistic Atomic Structure Package (GRASP) [1] for the ASOS community. To celebrate the 10<sup>th</sup> anniversary of the international collaboration on Computation Atomic Structure (CompAS) [2], a Special Issue of Atoms dedicated to GRASP was recently published [3].

The most important contribution to this issue is the GRASP manual describing the application of the package for evaluating various properties of atomic systems, supported by a paper that describes the underlying theory as it is implemented in the code. This complete documentation provides useful guides for new groups of users from the ASOS community to produce reliable atomic data that meet the accuracy requirements.

To illustrate the capacity of the GRASP package and the underlying role of the CompAS community in methodological and computational developments, new features of the code and recent extensions will be described, together with examples of calculations of relevance for astrophysics, plasma physics, and nuclear physics.

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