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LABORATORY DETERMINATION OF SPECTROSCOPIC DATA FOR STELLAR PHYSICS

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Abstract. Laboratory works on VUV emission spectra of moderately charged atomic ions aiming to obtain fundamental data needed for interpretation of observations are presented. Experimental and theoretical methods, as well as examples of studies are summarized.

1 Introduction

High resolution stellar spectra obtained by space instruments (HST/STIS, FUSE) in the far UV wavelength range need exhaustive laboratory spectroscopic data to be analyzed. In particular, improved data are necessary for complex spectra of heavy elements ions, such as moderately charged transition elements or rare earths, the presence of which were detected in chemically peculiar stars and white dwarfs. The precision on wavelengths needed for reliable identifications of species in the stellar spectra cannot be achieved by *ab initio* theoretical calculations but only by laboratory experimental measurements. For NLTE collisional-radiative modeling of stellar plasmas, a huge amount of spectroscopic and collisional data is needed, which implies the knowledge of experimental energy levels. These are derived from analysis of high resolution laboratory spectra in relation with theoretical studies of the atomic structure. The analysis also leads to a better knowledge of the quantum state wave functions, which provides better values of transition probabilities and Landé factors of the levels. Furthermore, experimental values of level energies enable improvement of calculations of photoionization cross sections or collisional excitation cross sections. In this report, we have limited the description of the experimental part to the vacuum ultra-violet (VUV) wavelength region. However, in some cases, we have to combine experimental data from different wavelength regions, either visible or infrared, produced by other authors. The theoretical method and analysis remain similar.

2 Experimental method

Several light sources are used in our laboratory for production of emission spectra of moderately charged atomic ions, depending on the ionization stages of interest. For instance, hollow cathode discharge sources operating in continuous mode produce emission of neutral atoms and singly ionized ions. In pulsed mode, they produce emission of doubly charged ions. Vacuum spark sources can produce emission of three to eight times charged ions, depending on the element constituting the anode.

For the VUV range, high resolution emission spectra are recorded on the 10.7 m normal incidence vacuum spectrograph of the Meudon Observatory (Tchang-Brillet & Azarov 2002). This high resolution instrument is unique in Europe and is registered in the ESA Ground Based Facilities (GBF) database. The instrument is equipped with a 3600 lines/mm holographic concave grating and has a linear dispersion of ~ 0.025 Å /mm operating in the 200-3000 Å wavelength region. The theoretical resolution is 150 000 (in practice $\delta\lambda \sim 0.008$Å). Two image plates or two photographic plates can be used to provide a simultaneous detection of a 200-240 Å wide wavelength range. The photo-stimulable image plates have a linear intensity response over five orders

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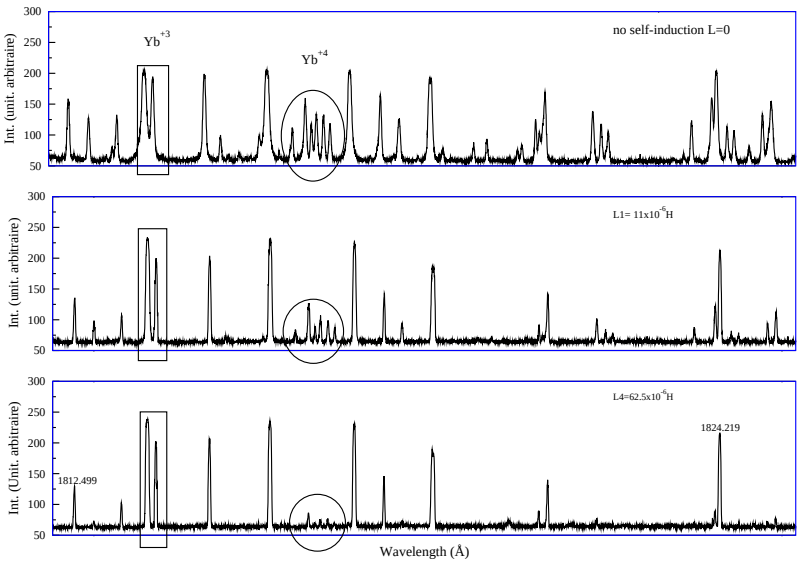

Fig. 1. Sections of spark spectra of an ytterbium electrode produced with three different discharge conditions. One can see the difference in behavior of Yb^{3+} and Yb^{4+} lines when the self-induction of the discharge circuit increases.

of magnitude and their use allows intensity measurements of spectral lines and comparison with theoretical oscillator strengths or branching ratios.

The grating instrument is complementary to high resolution Fourier Transform Spectrometry (FTS) (Tchang-Brillet & Azarov 2002). Indeed, given the absence of a transmitting device, it can be used at wavelength ranges shorter than the cut-off of the FTS beam-splitter. Moreover, its integrating operation mode allows a non-stationary or pulsed light sources, which is generally necessary for producing emission spectra of more than doubly charged ions.

3 Theoretical method

Theoretical calculations are performed using the set of Cowan's codes RCN/RCN2/RCG/RCE (Cowan 1981). In a first step, Hartree-Fock method is applied including corrections (HFR) using RCN/RCN2. Then the Hamiltonian including configuration interactions is diagonalized using RCG. In this step, the HFR energy parameters can be replaced by their scaled values. The scaling factors are provided by isoelectronic or isoionic regularities. The last code (RCE) introduces a semi-empirical step by allowing iterative least-squares fits of energy parameters, which minimize the standard deviation of calculated level energies from the experimental ones. The last iteration leads to the best calculated values of transition probabilities, Landé factors and experimentally unknown levels.

4 Analysis

The analysis consists of the derivation of energy levels from an experimental line list based on the Ritz combination principle taking into account quantum mechanical selection rules for electric dipole transitions. In practice, it is a long procedure involving manipulation of a large amount of experimental and theoretical quantities such as experimental wavelengths and intensities, calculated energies and line strengths, and going back and forth between these. This step has been greatly speeded up by using an interactive code IDEN (Azarov 1991, 1993) to visualize data. Finally, experimentally determined energy values are optimized by a general least squares fit from wave numbers of all observed lines using the LOPT code (Kramida 2010). These optimized experimental

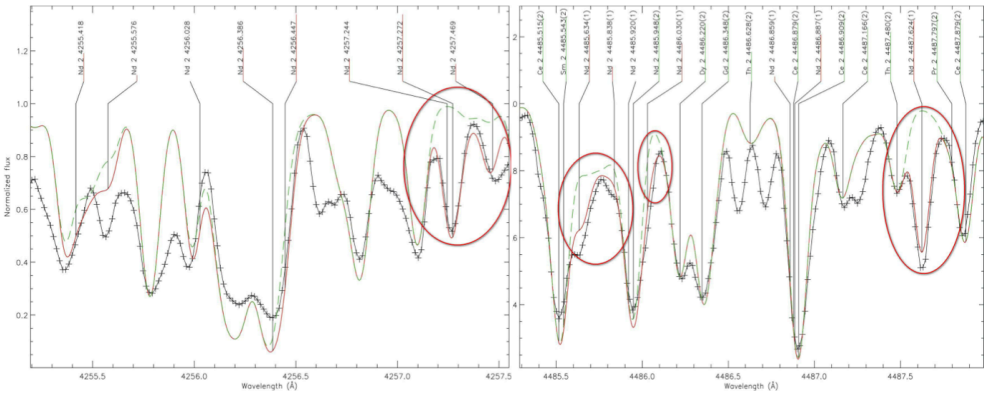

Fig. 2. Comparison between the observations (crosses), calculations with previous list of Nd II lines (dashed line) and new line list (full line)(Wyart et al 2010)

values are then used for computing Ritz wavelengths, which have reduced uncertainties compared with the directly measured wavelengths.

5 Typical results

In our laboratory, we have been working on spectra of moderately charged (II-VI) transition metal ions and rare earth element ions (lanthanides) for a longtime. The complexity of these spectra is due to the presence of incomplete d shell and f shell electrons. For rare earth ions, a systematic approach by isoelectronic or isoionic sequences must be followed to get reliable results. This allows simultaneously a critical compilation of existing data. Tables of our published data are made available online at `molat.obspm.fr` before being progressively included into databases like ADS (Kramida et al 2014) and Vienna Atomic Line Database (VALD 2014). Linelists contain experimental wavelengths and intensities, Ritz wavelengths calculated with optimized energies, calculated gf values, identifications of lower and upper levels of the transitions. Tables of energy levels contain level energies, quantum numbers, percentage compositions of levels in a given angular momenta coupling scheme and finally Landé factors. Most of the references of our previous works can be found on `molat.obspm.fr` as well as tabulated data. Works in progress concern spectra of manganese (II-V), iron and nickel ions, erbium ions Er^{2+} and Er^{3+}. The Meudon 10.7 m spectrograph is also used for studying rotationally-resolved electronic spectra of small molecules in VUV.

Figure 1 shows sections of high resolution spark spectra of ytterbium electrode, which have been used for the Yb V analysis (Meftah et al 2013). They are produced with different discharge conditions in order to differentiate lines from ionization stages.

Figure 2 shows a comparison between the spectrum of the Przybylski star (HD 101065) and two calculated spectra, one with data in VALD prior to our new analysis of the Nd II spectrum (Wyart et al 2010) and one with the newly included data. The new analysis resulted in the determination of 597 levels of the odd $4f^35d6s + 4f^35d^2 + 4f^36s^2 + 4f^46p + 5p^64f^5$ configurations and 233 levels of the even $4f^46s + 4f^45d + 4f^36s6p + 4f^35d6p$ configurations of the singly charged Nd^+ ion and it should increase the number of Nd II lines from 1287 to 5700 in VALD.

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