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Original software publication

ASAS: Computational code for Analysis and Simulation of Atomic Spectra

Jhonatha R. dos Santos [a,b,*], Luiz F.N. Barreta [a], Maria E. Sbampato [b], Marcelo G. Destro [b]

[a] Technological Institute of Aeronautics - ITA, 12228-900, São José dos Campos, SP, Brazil
[b] Institute for Advanced Studies - IEAv, 122280-970, São José dos Campos, SP, Brazil

A R T I C L E   I N F O

A B S T R A C T

The laser isotopic separation process is based on the selective photoionization principle and, because of this, it is necessary to know the absorption spectrum of the desired atom. Computational resource has become indispensable for the planning of experiments and analysis of the acquired data. The ASAS (Analysis and Simulation of Atomic Spectra) software presented here is a helpful tool to be used in studies involving atomic spectroscopy. The input for the simulations is friendly and essentially needs a database containing the energy levels and spectral lines of the atoms subjected to be studied.

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Software metadata

Current software version	Beta 1.0
Permanent link to executables of this version	https://github.com/ElsevierSoftwareX/SOFTX-D-16-00062
Legal Software License	GNU GPL version 3.0
Computing platform/ Operating System	Microsoft Windows (32 bits or 64 bits)
Installation requirements & dependencies	NET Framework 4.0 or superior
If available Link to user manual - if formally published include a reference to the publication in the reference list	https://github.com/JhonathaRicardo/ASAS/blob/master/ASAS%20MANUAL.pdf
Support email for questions	jhonatharicardo@gmail.com

1. Motivation and software description

Spectroscopy is the support science that allows the study of materials and processes by the observation of emission and absorption spectra of electromagnetic radiation. The atomic structure of an atom is unique, as is its emission or absorption spectrum. Thus, the knowledge of the atomic spectrum allows, for instance, the identification and measurement of an element concentration in a sample. This paper presents a tool for atomic spectra simulation, which optimizes experimental planning and helps in the analysis of experimental data. The computational code was specifically developed to be employed in spectroscopic studies, aiming laser isotopic separation process [1–3].

This computational code is named ASAS (Analysis and Simulation of Atomic Spectra). The ASAS version presented in this paper (current version, 013.0 [4]) was developed in Visual Basic and requires the Microsoft Windows system with the .NET framework 4.5 or superior. All graphics generated by ASAS were plotted using the Gnuplot graphics software [5], that is packaged and distributed with the ASAS code. It is important to emphasize that the Gnuplot license enables its distribution together with other software. This ASAS version has four functions. (i) Transitions From a Level: this function determines the possible energy transitions between the energy levels of a specific atom. In order to do that, this method applies selection rules for angular momentum and parity rules for the electric dipole moment. This simulation is performed considering transitions from an initial desired energy level to other

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energy levels; (ii) Possible Transitions: if the user does not specify an initial energy level, this function defines all the allowed energy transitions within a spectral range; (iii) Spectra Simulation: this function simulates spectra considering a Lorentzian profile in order to simulate the curves; and finally (iv) the Electronic Temperature function performs the calculation of the electron temperature using the Boltzmann plot method. This method determines the electronic temperature using the intensity of different lines found in the experimental atomic spectra [6].

Currently, the ASAS has been used in projects developed in the Institute for Advanced Studies (IEAv) in Brazil [6,7]. More information on software installing are found in its manual [4].

2. Framework software: Functions and database

This section describes the functions and database of ASAS software. The details of each function, database and symbols shown below can be found in the program manual [4].

2.1. Database

The default database set for the ASAS was developed for the PASIL project (in Portuguese, *Processo Atômico de Separação Isotópica a Laser*) carried out in the Photonics Division of the Institute for Advanced Studies (IEAv) [8]. The diversity of atoms studied in our group requires an organization of the data for each atom. The spectroscopy data in the PASIL data based are taken from the National Institute of Standards and Technology (NIST) database. Further, the PASIL database follows the NIST database format.

The NIST file format used in PASIL enables the inclusion by the user of information about other atoms in the database. The PASIL database is divided into two file directories. The first one is related to the spectral lines data and the second contains information about the energy levels [4]. The database of the current ASAS version includes data of a few neutral atoms (Ar I, Ne I, Dy I, Mo I, Ti I, Er I and Nd I) extracted from the literature [9,10]. Details about formatting and building of the database files can be found in the ASAS manual [4].

2.2. Function to determine transitions from a level

The first ASAS function determines the Transitions from a Level. This function identifies the allowed electronic transitions from a particular level, within a given spectral range. In order to do that, the ASAS performs a scan of the energy levels in the database, applying the selection rules for total angular momentum and parity. There will be only transitions between energy levels that have different parity (odd–even or even–odd parity), and between levels which have total angular momentum difference to 0 or ± 1 [11]. This function checks if the transition is listed in the database and the results are provided to the user through a data table.

2.3. Function to determine possible transitions

The ASAS software defines "possible transitions" as all allowed transitions, whether or not the transitions are experimentally observed in the literature [9,10].

The Possible Transitions function uses the database of energy levels to calculate all allowed transitions within a spectral range, applying the selection rules in the same way as in the previous function (Transitions from a Level). However, the search is not restricted to one level [11], i.e. the calculation of the transitions are performed starting from any initial energy level to any other energy level. This function is designed to assist the user to identify lines in experimental spectra and the results are provided in a table. The simulations are limited to a range of 10 nm due to a large number of possible transitions generated by this kind of search.

2.4. Function for spectra simulation

The Spectra Simulation function uses the database and input parameters to build simulated atomic spectra with Lorentzian curves profiles.

The experimental absorption or emission spectra do not show strictly monochromatic lines. Each spectral line is observed as an intensity distribution around a central resonance frequency. This phenomenon is the result of the multiple lines broadening process [12,13]. One specific absorption or emission line is described by an intensity distribution function I depending on the wavelength, λ:

$$I(\lambda) = \frac{\delta\lambda}{2\pi} \frac{1}{\left(\frac{\delta\lambda}{2}\right)^2 + (\lambda - \lambda_0)^2} \tag{1}$$

where: $\delta\lambda$ is the full-width at half-maximum (FWHM) and λ_0 is the central wavelength of the transition.

In summary, the user defines the spectral range, the atom and the FWHM. From these parameters, ASAS checks the contribution of each of the lines present in the simulation range at each wavelength of the spectrum, considering a Lorentzian line profile. Unlike other ASAS functions, the Spectral Simulation function allows the user to build spectra of atoms that are not included in the software database.

2.5. Electronic temperature function

The Electronic Temperature function uses the database and the intensities of experimental spectra to determine the electron excitation temperature of a system using the Boltzmann plot method [14–16], which is considered one of the best diagnostic methods to estimate electronic temperature. From the atomic emission spectroscopy theory, the relationship between the relative intensities of spectral lines, and the electronic temperature is obtained from Eq. (2) [14,17]:

$$ln\left(\frac{I_{ul}\lambda_{ul}}{g_u A_{ul}}\right) = C - \frac{E_u}{k_B T_e} \tag{2}$$

where I_{ul} is the spectral line intensity, λ_{ul} is the transition wavelength, g_u is the statistical weight of the electronic state, A_{ul} is the Einstein emission coefficient, k_B is the Boltzmann constant, T_e is the electronic temperature and C is a constant terms of the equation. The indices u and l correspond respectively to the upper and lower energy levels (E_u and E_l) of each electronic transition.

With the appropriate number of spectral lines a plot of the logarithmic function, $ln(I_{ul}\lambda_{ul}/g_u A_{ul})$, is built as a function of the upper energy level, E_u. The electronic temperature is determined by the slope of a linear fit of the curve. The quality of the fit is given by the coefficient of determination R^2. The value of R^2 ranges from 0 to 1 with a higher value indicating a better quality fit. For this purpose, it is considered a good correlation if $R^2 > 0.81$ [14].

The Boltzmann plot method is also applied to absorption spectra. The process is similar to that performed for emission spectra. However, the electronic temperature is calculated using Eq. (3) [15],

$$ln\left(\frac{A}{g_l B_{lu}}\right) = C - \frac{E_l}{k_B T_e} \tag{3}$$

where A is the absorbance of each line under study, B_{lu} is the Einstein absorption coefficient and E_l is the lower energy level.

The distribution of the electron population is given by Eqs. (4) and (5):

$$N_l = \frac{N_T g_l}{Z} exp\left(\frac{-E_l}{k_B T_e}\right) \tag{4}$$

$$Z(T_e) = \sum_j g_j exp\left(\frac{-E_j}{k_B T_e}\right) \tag{5}$$