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NIST atomic spectra database

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Abstract. Accurate atomic data have great importance in astrophysics, plasma research, and other fields of physics. For more than 10 years, the Atomic Spectra Database (ASD) at the National Institute of Standards and Technology has served as a convenient and robust source of critically evaluated data on tens of thousands of spectral lines and energy levels. The recent upgrade of the ASD represents a significant new step in the development of dynamic databases providing powerful tools for data analysis and manipulation. We present a detailed description of ASD 3.0 emphasizing numerous advanced features and options for data search and presentation.

Key words. Atomic data – Atomic processes – Plasmas

1. Introduction

The extensive utilization of atomic data in physics, astrophysics, atmospheric science, and other fields of research stimulates production of both accurate data sets and new tools for data dissemination. It is no surprise, therefore, that we currently observe significant improvements in the accuracy of theoretical calculations and experimental measurements along with actively pursued programs on the development of atomic databases, especially Internet-based ones.

The National Institute of Standards and Technology (NIST) supports the Physical Reference Data Program which provides data on fundamental physical constants, atomic and molecular spectroscopy, ionization cross sections, absorption of x-rays and gamma rays, radiation dosimetry, half-life measurements, atomic weights, and condensed matter physics. The NIST online databases containing those data are actively used by many thousands of researchers who appreciate both the quality of data and the user-friendly interface of the databases.

Critical assessment and dissemination of atomic spectroscopic data occupy an important place in the list of activities at NIST. New compilations of atomic data are regularly published in various journals, and new specialized databases appear quite frequently. Nevertheless, the largest and most extensive of the NIST atomic databases, the Atomic Spectra Database (ASD), has not been upgraded since late 1990s, and it is only very recently that the latest version (ASD 3.0) became publicly accessible on the Web.

Although generally upgrading of databases is considered to be a routine operation, ASD 3.0 represents a qualitatively new development. It was built using the latest advancements in database management, and it involves modern user interface features and advanced computer technologies. Here we present a detailed description of ASD 3.0

along with some illustrative examples of database operation and data presentation. ASD 3.0 can be freely accessed at the URL `http://physics.nist.gov/asd/`.

2. Database Organization

The core of ASD 3.0 is the open-source MySQL[1] relational database management system (RDBMS) that is used by millions of users worldwide. MySQL has a number of features that are highly important for the development of the ASD. First of all, this RDBMS is very reliable and stable. It also provides a cross-platform support, which is crucial for our work since the ASD is developed on a Linux server while the release version runs on an AIX workstation. Another important feature includes very rich options for interaction with Internet applications. Finally, as an open-source software, MySQL can be freely upgraded to the latest versions of the RDBMS.

Usage of an RDBMS allows us to significantly improve consistency and integrity of atomic data, such as, for instance, unambiguous correspondence between the energy levels and related spectral lines. Currently the ASD provides a partial integration of numerical and bibliographic data, and we plan to reach a completely integrated mode in the future versions.

For ASD 3.0 the WWW user interface was totally rewritten. It is now based on a library of Perl scripts and open-source graphical software and includes a newly developed help system using popup windows. The entry form page for energy levels is shown in Fig. 1.

3. Available Data

The unique feature of the ASD that distinguishes it from virtually all other existing spectroscopic databases is that all data in the ASD have been critically evaluated and assessed. The amount of spectroscopic data available in ASD 3.0 has been considerably enlarged. As of mid-2005, there are more than 75,000 energy levels for 58 elements and 125,000 spectral lines for 99 elements with approximately 44,000 lines having data on transition probabilities. This represents a 30% increase in the number of spectral lines and almost 10% increase in energy levels compared to the previous version of the ASD. The list of the most represented elements is given in Table 1. It should also be mentioned that the use of an RDBMS significantly facilitates the addition of spectroscopic data, so that the new data compilations published by the NIST Atomic Spectroscopy Group staff are almost immediately added to ASD.

ASD 3.0 provides a very detailed version history including a list of corrected misprints, information about new data, and even explanations on data accuracy assessment and evaluations. The most important recent data additions to ASD 3.0 are the following:

- spectral data for highly-charged ions of Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo (Shirai et al. 2000),
- spectral data for astrophysically important ions of Ne, Mg, Si, and S (Podobedova et al. 2003, 2004a,b,c),
- spectral data for Ba I-II (Curry 2004), Zr III-IV (Reader & Acquista 1997a,b), W I-II (Kramida & Shirai 2005), Ne I (Saloman & Sansonetti 2004)
- data on energy levels and spectral lines for all ionization stages of Xe I-LIV (Saloman 2004) and Rb I-XXXVII (Sansonetti 2005).

In the near future, new data on ions of Ne, W, Ga, Fe, and other elements important for astrophysics and plasma diagnostics will be added to the database.

4. Main Search, Selection, and Output Options

The previous versions of the ASD provided a significant number of search, selection and output (SSO) options to choose from. ASD 3.0 adds several new features, including graphical ones, which are discussed in Section 5.

[1] Any mention of commercial products is for information only; it does not imply recommendation or endorsement by NIST.

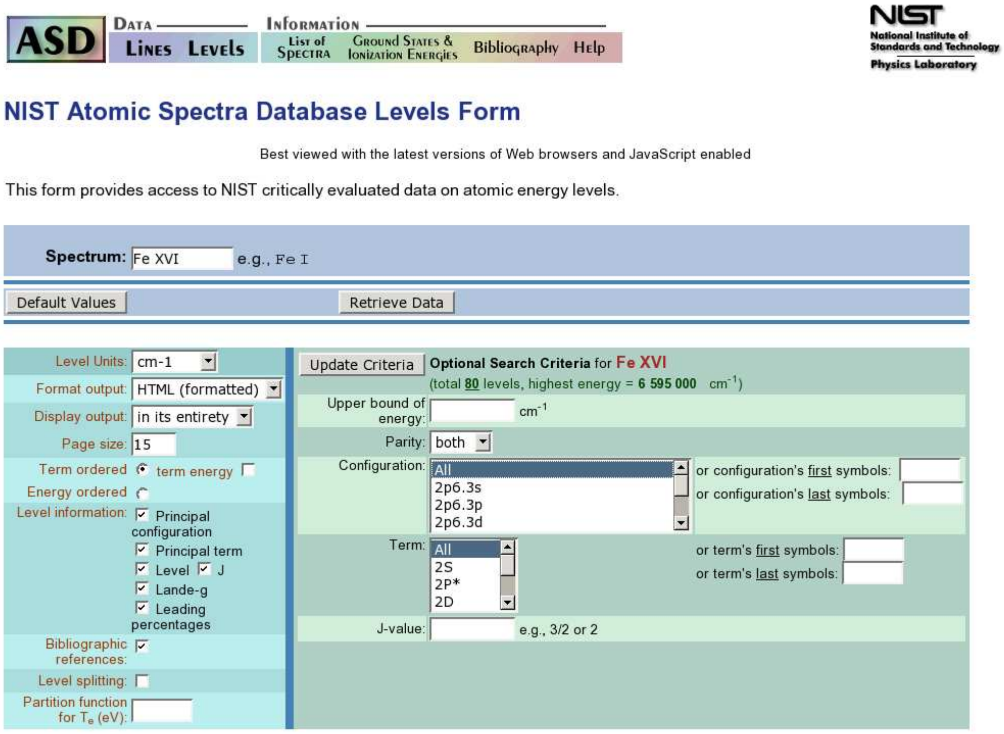

Fig. 1. ASD 3.0 entry page for energy levels.

Table 1. The most represented elements in the ASD with the total number of levels greater than 2000 or total number of lines greater than 5000. The number of lines or levels is given in parentheses.

Levels	**Fe** (3474), **Ni** (2974), **Cr** (2606), **Mn** (2556), **Cu** (2544), **Co** (2432), **V** (2064), **Mo** (2026)
Lines	**W** (9887), **Fe** (7180), **O** (5773), **Xe** (5758), **Sc** (5088)

Figure 1 shows the complete set of options for querying the energy levels. The levels are shown for a single ion, and one can restrict the output to a predetermined set of configurations, terms, J-values, or, for instance, such parameters as level multiplicity or upper bound of energy. One can use different units for the energy output, different formats (HTML or ASCII), and different ordering of levels, i.e., strict energy ordering or grouping by terms. In the latter case, the average term energy can be calculated online as well. By deafult, complete information on level quantum numbers is printed, although some or all parameters may be deselected for the printout.

The last three options for the energy level queries are new in ASD 3.0. First, a set of bibliographic references can be requested and browsed in a small popup window. Also, a user may request an extra column containing differences between adjacent energy levels to be displayed. Finally, a partition function for an

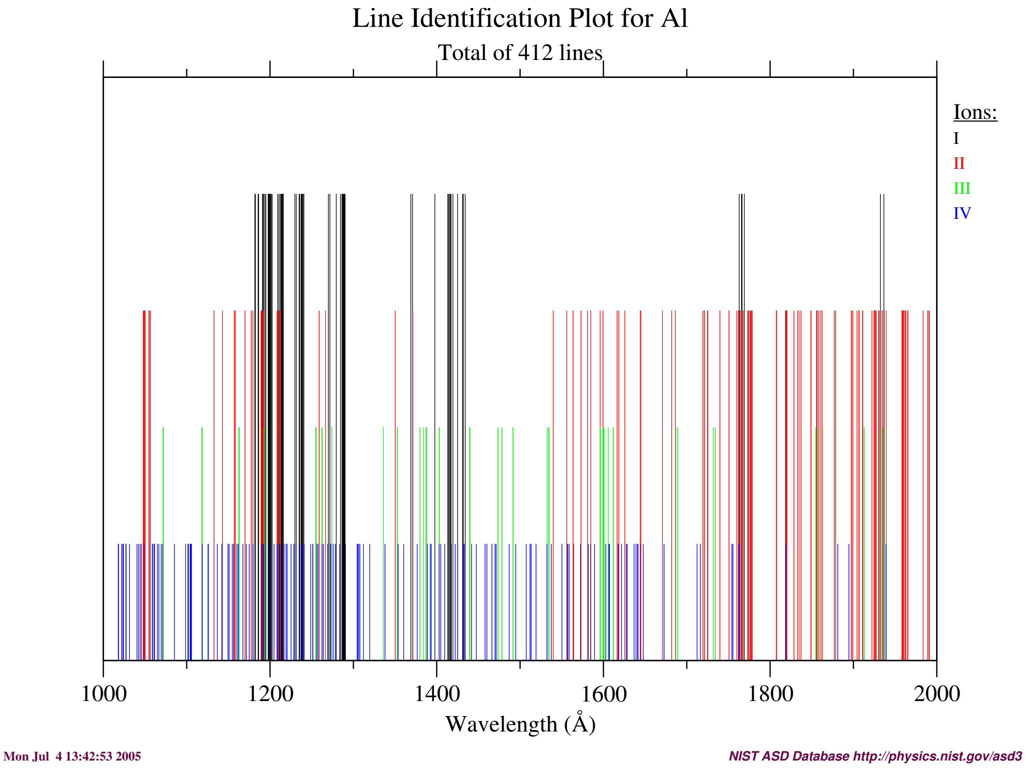

Fig. 2. Line identification plot for ions Al I-IV.

arbitrary value of electron temperature can be calculated online.

The existing broad set of SSO options for spectral line queries in the ASD, including transition probabilities and accuracies, was extended to include such features as multiplet grouping of transitions and output of bibliographic references for lines and transition probabilities. The most important additions, however, involve the graphical presentation of data.

5. New Graphical Capabilities

Although online atomic spectroscopic databases have been available at NIST since mid-1990s, it is ASD 3.0 that provides, for the first time, new dynamic graphical capabilities. The data plots are generated in various formats, including PDF and PNG, and the actual numerical data are given in tabular form as well. Below we briefly outline those new feaures and present some examples.

5.1. Line Identification Plot

These plots show *positions* of spectral lines for one or several ions of the same element within a specific wavelength range. An example showing the distribution of 412 lines for Al I-IV in the range of λ = 1000 Å to λ = 2000 Å is presented in Fig. 2. This feature was developed by a direct request from experimentalists to assist in quick identification of measured lines. The lines from each ion are represented by vertical lines of the same color and height, which allows easy recognition, as can be seen from Fig. 2.

5.2. Saha-LTE Plot

This option allows a user to calculate a Saha-LTE line emission spectrum for arbitrary val-

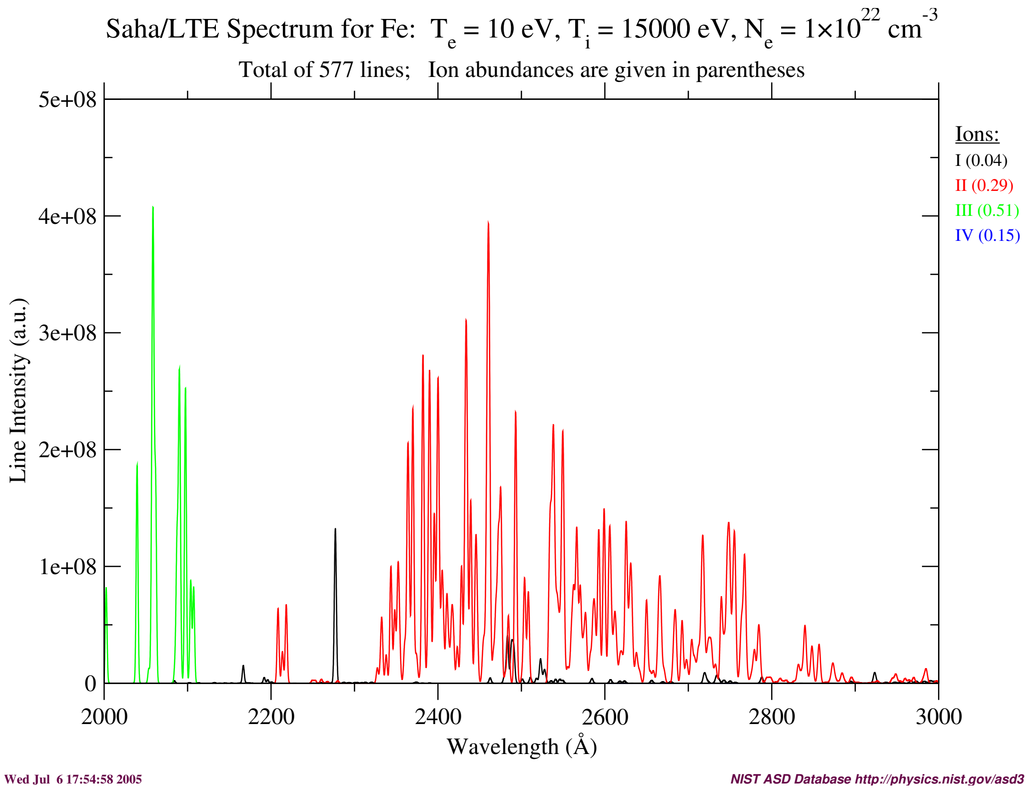

Fig. 3. Plasma emission spectrum for Saha-LTE equilibrium, $N_e = 10^{22}$ cm^{-3}, T_e = 10 eV. The ions included are Fe I to Fe IV. The ionization composition is shown on the plot.

ues of electron temperature T_e and density N_e with or without Doppler broadening. As ASD 3.0 does not contain any collisional data, we are currently restricted to the Saha-LTE equilibrium only, although extensions towards coronal or collisional-radiative equilibria are currently under discussion. To generate the spectrum, a user is required to input the spectral range, T_e, N_e, ion temperature T_i, and the number of points. The populations of atomic levels are determined from the Saha-Boltzmann formulas, and the spectrum is calculated assuming the plasma to be optically thin. As Doppler broadening depends on T_i, which is an independent input parameter, it can also be used to simulate effects of instrumental broadening, and thus the spectra can be directly used in applications.

An example of a Saha-LTE plot is presented in Fig. 3. A total of 157 lines from ions Fe I to Fe IV between 2000 Å and 3000 Å are shown for plasma conditions of $N_e = 10^{22}$ cm^{-3}, T_e = 10 eV, and T_i = 15 keV. As can be seen from the Figure, the most abundant ion is Fe III having about 51% of the total ion population.

5.3. Grotrian Diagrams

ASD 3.0 implements dynamic generation of Grotrian diagrams for arbitrary ions. The Java applet shows the positions of all energy levels and the radiative transitions between them on a correct energy scale, thereby providing a convenient and clear visualization of the whole energy structure for a particular ion including ionization energies (Fig. 4). Practically all basic information on levels and lines can be obtained by a mouse click. For instance, when

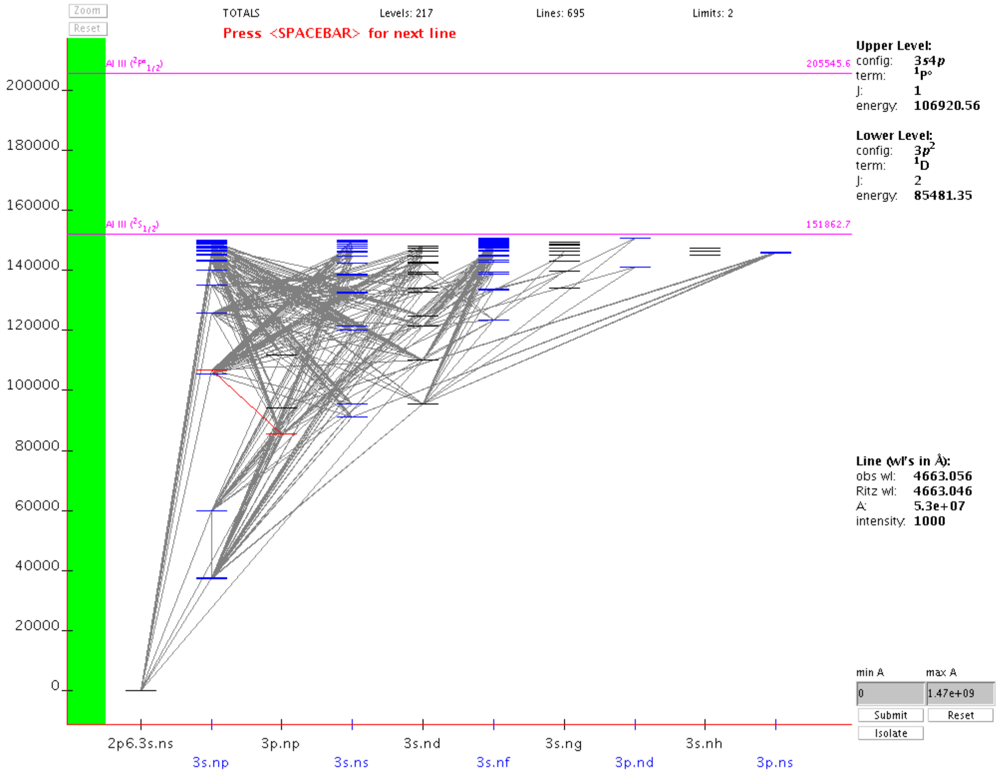

Fig. 4. Dynamically generated Grotrian diagram for Al II. There are total of 217 energy levels, 695 spectral lines, and 2 ionization limits on this plot.

a user selects a level, such information as its energy and quantum numbers (configuration, term, angular momentum) are displayed on the diagram. Selecting a spectral line results in display of the same information for both lower and upper levels, and, in addition, observed and/or calculated wavelengths, transition probability, relative intensity, accuracy. The selected objects, i.e., line and/or level(s), are highlighted in red for easier recognition, as can be seen from Fig. 4.

The Grotrian Java applet allows one to perform various search and selection operations. The green band next to the energy axis is used to zoom particular parts of a spectrum. The ”minA” and ”maxA” fields permit one to filter out spectral lines with small or large values of transition probability. Also, one can study radiative transitions from or onto a specific level using the ”Isolate” button. Other options, e.g., grouping by configuration or term multiplicity, are available from the lines query page.

6. Future Plans

The new version of the NIST Atomic Spectra Database exemplifies a new approach to development of atomic databases at NIST. ASD 3.0 is based on a modern relational database management system, involves advanced computer technologies, and provides a user-friendly access to a variety of critically evalulated atomic parameters. Future versions of ASD will reach a complete integration of numerical and bibliographic data. We also plan to add new powerful tools for calculation of plasma emissivities and ionization balance under diverse conditions. Most importantly, new compilations of critically evaluated atomic spectroscopic data will be regularly added to the NIST Atomic

Spectra Database thereby providing more assistance to research in astrophysical and laboratory plasmas.

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