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Atomic Spectroscopic Databases at NIST

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ABSTRACT

We describe recent work at NIST to develop and maintain databases for spectra, transition probabilities, and energy levels of atoms that are astrophysically important. Our programs to critically compile these data as well as to develop a new database to compare plasma calculations for atoms that are not in local thermodynamic equilibrium are also summarized.

The NIST Physics Laboratory provides a number of atomic spectroscopic databases on the World-Wide-Web that are widely used in astrophysics. The data consist mainly of wavelengths, energy levels, and oscillator strengths that have been critically evaluated in the NIST Atomic Spectroscopy Data Center. These data play an important role in line identification, spectra modeling, and other astrophysical research. All databases can be accessed from the NIST Physics Laboratory home page <http://www.physics.nist.gov>, select Physical Reference Data.

Since the last Workshop, some of the existing databases were significantly expanded, and a number of new databases became available on the Web. The NIST **Atomic Spectra Database** (ASD) has been upgraded from version 2.0 to 3.0. It now contains detailed information on more than 75,000 energy levels and almost 130,000 spectral lines for ions of 99 elements. New large sets of data were recently added for the spectrum lines and energy levels of Ne I, Hg I and II, Be II, Xe and Rb in all ionization stages, highly-charged ions of the iron period of elements, Cu, Mo, and Kr (taken from Mon. 8 of J. Phys. Chem. Ref. Data), Zr III and IV, Ba I and II, and W I and II. Data for the transition probabilities of Ba I and II were also added.

Our program to carry out critical compilations of the spectra, transition probabilities, and energy levels of atoms of astrophysical interest also continues actively. A major reassessment of transition probabilities for Fe I and II (W. Wiese and J. Fuhr) has been completed

and is in press at the Journal of Physical and Chemical Reference Data (JPCRD). Recent work on transition probabilities for neutral and singly ionized C, N, and O is described in an accompanying paper by W. Wiese and J. Fuhr in these proceedings. Work on Na and Mg in all stages (D. Kelleher and L. Podobedova) is now in press at JPCRD and new compilations for Si and Al (D. Kelleher and L. Podobedova) will be submitted shortly.

For wavelengths and energy levels, a compilation of Kr in all stages of ionization (E. Saloman) is now in press at JPCRD as are compilations for Hg I (E. Saloman), and Rb in all stages (J. Sansonetti). The data for Hg I and Rb have already been added to ASD, and the addition of the data for Kr is now in progress. A compilation of Cs spectra in all stages (J. Sansonetti) is nearing completion. Similar compilations for Na, K, and Fr are in progress (J. Sansonetti). The compilations for alkali metals include transition probabilities, where available. An extensive compilation for Ne I (E. B. Saloman and C. Sansonetti) was recently published in JPCRD. Works on Ne II (A. Kramida and G. Nave) and Ne VIII (A. Kramida and M.-C. Buchet-Poulizac) are in press at the European Journal of Physics. Compilations for Ne III (A. Kramida and G. Nave) and Ne VII (A. Kramida and M.-C. Buchet-Poulizac) have already appeared in that journal. A compilation for W I and W II (A. Kramida and T. Shirai) was recently published in JPCRD, and work on the higher stages of W (A. Kramida and T. Shirai) will be submitted to JPCRD shortly. Also in press at JPCRD is work on Ga in all stages (T. Shirai, J. Reader, A. Kramida, and J. Sugar). A compilation for Be II (A. Kramida) was published recently in *Physica Scripta*. Work on B II and B III (A. Ryabtsev, I. Martinson, and A. Kramida) is in progress. A compilation of Ar in all stages (E. Saloman) is also in progress.

We have recently implemented a new relational database management system that allows a high level of data integration and consistency. Its innovative user interface provides convenient access to various parameters. Several new additions to the ASD interface should be of special value to astrophysicists. Among those is the online Saha-LTE spectrum generation tool, which allows calculation of plasma emission spectra under Saha-LTE equilibrium for user-defined values of electron density and temperature. The calculated spectrum can also be Doppler-broadened for arbitrary values of ion temperature. This also may be used for simulation of instrumental broadening. Fig. 1 shows a synthetic spectrum for ions of Fe with wavelengths calculated from the known energy levels and intensities as calculated for an electron temperature of 8 eV, an ion temperature of 1000 eV, and an electron density of $1 \times 10^{22} \text{ cm}^{-3}$. As can be seen, under these conditions the spectrum is dominated by lines of Fe II.

Another feature of the new graphical interface is the availability of Grotrian diagrams. These diagrams provide an intuitive visualization of the atomic energy level structure and transitions, as well as direct access to the fundamental atomic data (energy levels, wavelengths, transition probabilities). Fig. 2 shows a Grotrian diagram for Na I constructed in real time from data in the database.

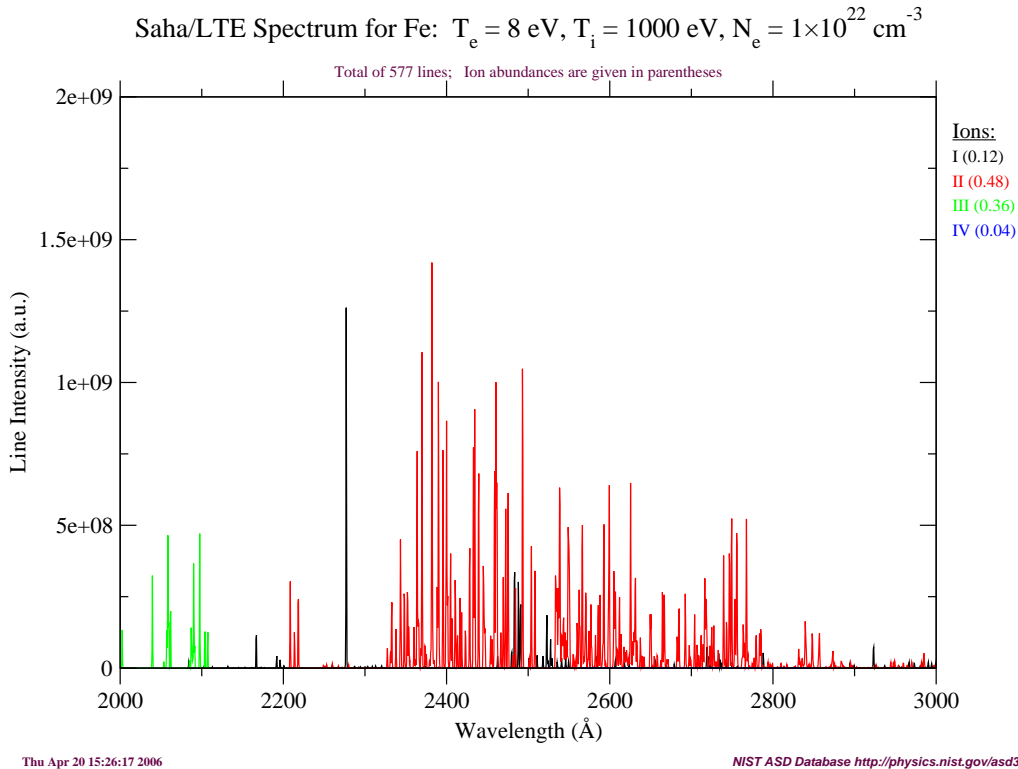


Fig. 1.— NIST ASD Database: Saha/LTE spectrum for Fe I-IV at electron density 10^{22} cm^{-3} and electron temperature 8 eV.

In recent years, three new databases became available. The first, **Handbook of Basic Atomic Spectroscopic Data**, now upgraded to v.1.1, provides the most frequently used atomic spectroscopic data in an easily accessible format. It includes data for the neutral and singly-ionized atoms of all elements hydrogen through einsteinium ($Z = 1-99$). Wavelengths, intensities, line classifications, and transition probabilities are given in a separate table for each element. The data for 12,000 lines of all elements are also collected into a finding list sorted by wavelength. This has now appeared as a journal paper in the JPCRD.

The second, **Spectral Data for the Chandra X-ray Observatory**, contains critically compiled wavelengths, energy levels, line classifications, and transition probabilities for ionized spectra of neon (Ne V to Ne VIII), magnesium (Mg V to Mg X), silicon (Si VI to Si XII), and sulfur (S VIII to S XIV) in the 20 \AA to 170 \AA region. These tables provide data of interest for the Emission Line Project in support of analyses of astronomical data from the Chandra X-Ray Observatory. The transition probabilities were obtained mainly from recent sophisticated calculations carried out with complex computer codes. These data have also appeared as journal papers in JPCRD.

The third is our **SAHA Plasma Population Kinetics Database**. This database

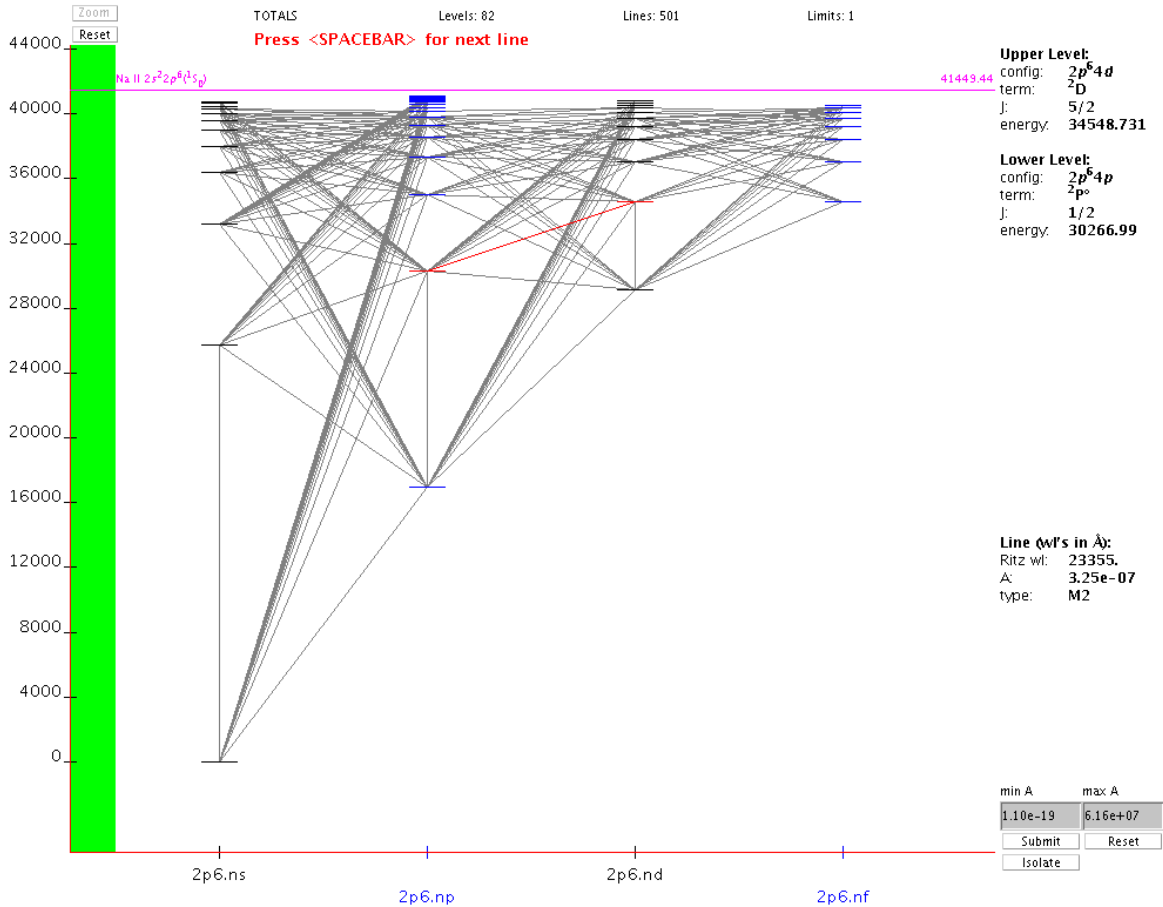


Fig. 2.— NIST ASD Grotrian diagram for radiative transitions in Na I.

provides benchmark theoretical results for population kinetics of various plasmas under non-local-thermodynamic-equilibrium conditions. Results of the 3rd Non-LTE Code Comparison Workshop held at NIST in December 2003 are given there. Parameters available for comparisons include mean ion charge, ion populations, synthetic spectra, and rates of collisional and radiative processes. The database will be complemented by a collisional-radiative code to allow online calculations in real time.

Work continues on our bibliographic databases for atomic transition probabilities and spectral line broadening, as well as our database on electron impact ionization cross sections. We expect our bibliographic database on energy levels and spectral lines to be available in the near future.

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