Atomic Spectroscopic Databases at NIST

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Abstract

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: 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.

A new relational database management system allows a high level of data integration and consistency, while the 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. Another example of a new graphical interface is the availability of Grotrian diagrams. This provides 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).

In recent years, two new databases became available. The "Handbook of Basic Atomic Spectroscopic Data," now upgraded to v.1.1, provides

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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. "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 to 170 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.

Work continues on the bibliographic databases for atomic transition probabilities and spectral line broadening, as well as the 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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