

NIST Atomic Spectra Database

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Version 1 of the NIST Atomic Spectra Database became available online as an interactive Web server in 1995. It is accessible at the NIST Physics Laboratory Web site (physics.nist.gov, select Physical Reference Data). Version 1 has data on atomic energy levels for some 500 spectra, transition probability data for spectra of the iron-group elements, and comprehensive wavelength data for spectra of several elements. It includes no data for one or more of these three types of data for many important spectra, however.

Pending new critical compilations of the most needed data, we are extending the database by editing and adding data from earlier NIST compilations, selected non-NIST compilations, and selected recent publications or unpublished material. The new Version 2 (hereafter referred to as “ASD”) contains significantly more data on atomic and ionic transitions and energy levels. It should be available on the Web within a few months. ASD has data for about 950 spectra, with about 70,000 energy levels and 90,000 lines, 40,000 of which have transition probabilities.

The data available in both Versions 1 and 2 are indicated according to spectrum in Figures 1, 2, and 3. The additional energy level data in Version 2 (Fig. 1) are largely taken from material compiled by R. L. Kelly in connection with his wavelength tables [1]. The additional transition probability data (Fig. 2) include new NIST compilations for the C, N, and O spectra [2], and data from other, mostly earlier, NIST compilations [3, 4, 5, 6]. In addition to wavelengths compiled in connection with transition probability data, extensive wavelength data for the first five spectra of many elements are included from the tables of Reader *et al.* [7] (Fig. 3).

Version 2 thus has energy level data for most spectra of H through Kr ($Z=1-36$), Mo ($Z=42$), and for 65 spectra of the rare-earth elements La through Lu ($Z=57-71$). Wavelengths of observed

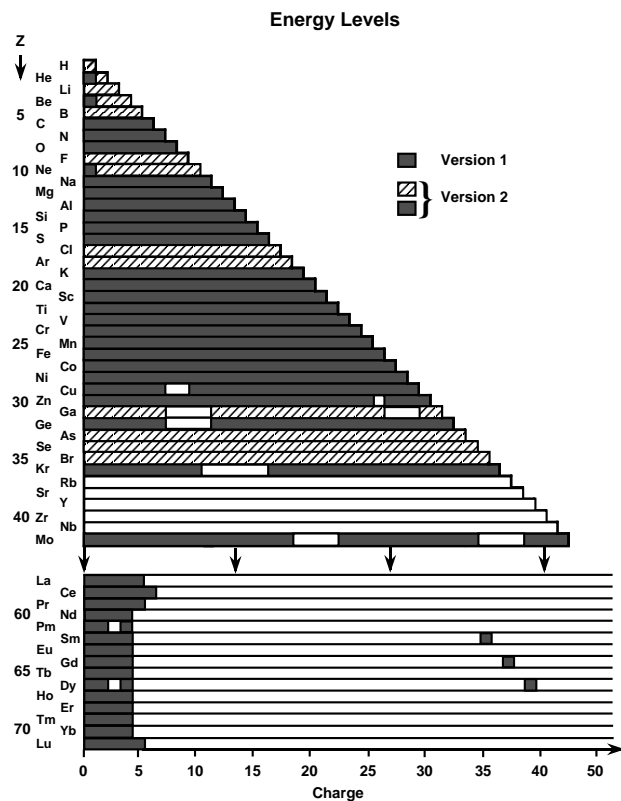


Figure 1: Holdings of energy-level data in Versions 1 and 2 of the NIST Atomic Spectra Database.

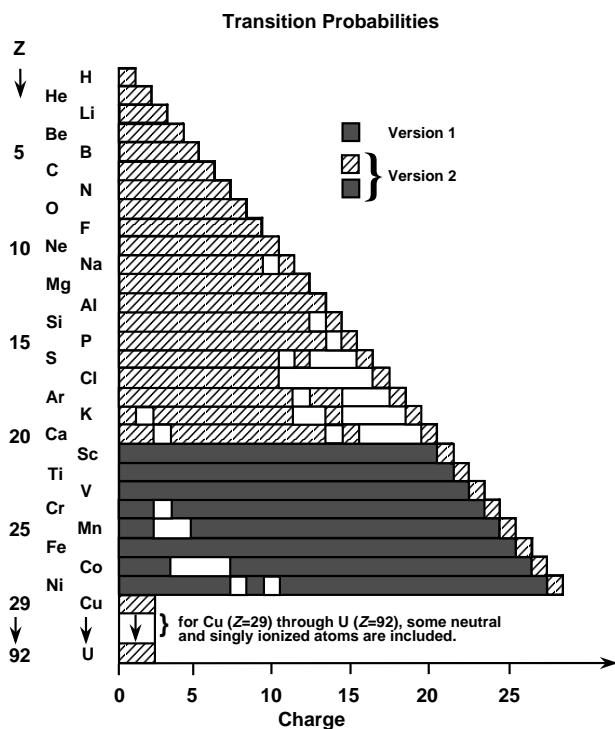


Figure 2: Holdings of transition-probability data in Versions 1 and 2 of the NIST Atomic Spectra Database.

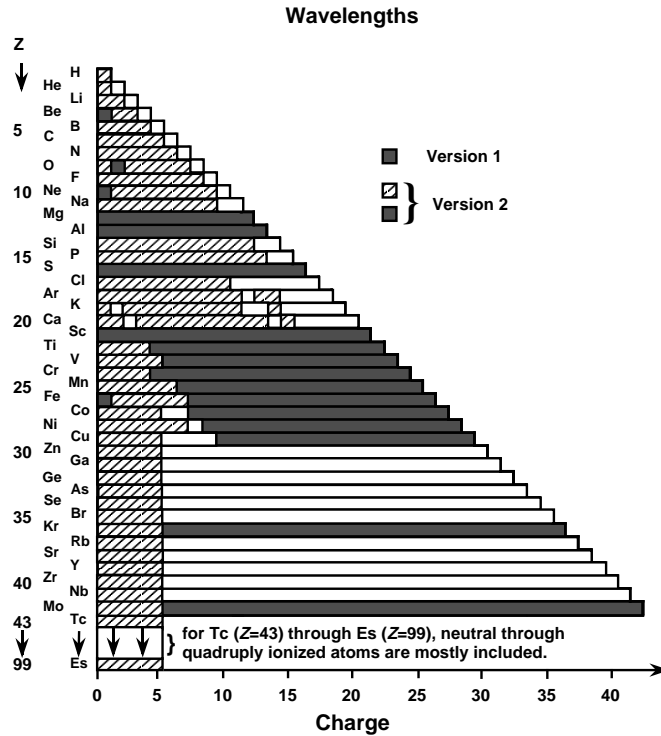


Figure 3: Holdings of wavelength data in Versions 1 and 2 of the NIST Atomic Spectra Database.

transitions are included for 99 elements. Energy-level classifications and transition probabilities are included for the lines of most spectra of H through Ni ($Z=1-28$). Comprehensive lists of observed wavelengths with classifications based on critically compiled level data are available for some elements, including all spectra of Mg, Al, S, and Sc. Wavelengths without level classifications are included for prominent lines of up to the first five spectra of Cu through Es ($Z=29-99$), with selected transition probabilities for the first two spectra. Several extensive data sets from recent NIST compilations are being prepared for inclusion in the database during the next year.

The two broad categories of queries handled by ASD are for data on energy levels and for data on spectral lines. The data are displayed in formats similar to those in NIST print publications of atomic spectroscopic data. In addition to graphical user interface format, users can choose output in an ASCII form easily read by spread-sheet software. ASD offers a range of user-specified options and selection criteria, each with its own default. For example, for transition strengths one may choose to search or display any combination of transition probability, oscillator strength, line strength, $\log(gf)$, and relative intensity. One may also choose from a variety of units and selection criteria on transition-strength accuracy and properties of energy levels. Outputs for transitions may be ordered by wavelength or by multiplets for a particular spectrum.

The database search programs for ASD are written in ANSI C and are thus portable to any environment, including PC's and UNIX-based machines. Only the graphical user interface for input/output is platform-specific. ASD comes with a built-in character-based interface, which itself is platform independent, and thus facilitates its inclusion in other character-based environments such as ALADDIN. In addition to the Web version, a PC version with a Windows interface will be made available on diskettes for purchase. This will replace the currently available DOS version.

Acknowledgements

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References

- [1] R. L. Kelly, "Atomic and Ionic Spectrum Lines Below 2000 Å: Hydrogen through Krypton," *J. Phys. Chem. Ref. Data* **16**, Supplement 1 (1987)
- [2] W. L. Wiese, J. R. Fuhr, and T. M. Deters, "Atomic Transition Probabilities of Carbon, Nitrogen, and Oxygen," *J. Phys. Chem. Ref. Data* Monograph 7 (1996)
- [3] W. L. Wiese, M. W. Smith, and B. M. Glennon, "Atomic Transition Probabilities (H through Ne—A Critical Data Compilation," *Natl. Stand. Ref. Data Ser.*, Natl. Bur. Stand. (U.S.) 4, Vol. I (1966)
- [4] W. L. Wiese, M. W. Smith, and B. M. Miles, "Atomic Transition Probabilities (Na through Ca—A Critical Data Compilation," *Natl. Stand. Ref. Data Ser.*, Natl. Bur. Stand. (U.S.) 22, Vol. II (1969)
- [5] *NIST Atomic Transition Probability Tables*, J. R. Fuhr and W. L. Wiese, in "CRC Handbook of Chemistry and Physics," 77th Edition, D. R. Lide, ed., p. 10-128 – 10-186, CRC Press, Boca Raton, FL 1996
- [6] *Atomic Spectroscopy*, W. C. Martin and W. L. Wiese, in "Atomic, Molecular, and Optical Physics Handbook," G. W. F. Drake, ed., Ch. 10, p. 135-153, AIP Press, New York 1996
- [7] J. Reader, C. H. Corliss, W. L. Wiese, and G. A. Martin, "Wavelengths and Transition Probabilities for Atoms and Atomic Ions, Part I. Wavelengths, Part II. Transition Probabilities," *Natl. Stand. Ref. Data Ser.*, Natl. Bur. Stand. (U.S.) 68 (1980)