NIST Databases on Atomic Spectra

J. Reader, W. L. Wiese, W. C. Martin, A. Musgrove, and J. R. Fuhr National Institute of Standards and Technology, Gaithersburg, MD

The NIST atomic and molecular spectroscopic databases now available on the World Wide Web through the NIST Physics Laboratory homepage include Atomic Spectra Database, Ground Levels and Ionization Energies for the Neutral Atoms, Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration, Bibliographic Database on Atomic Transition Probabilities, Bibliographic Database on Atomic Spectral Line Broadening, and Electron-Impact Ionization Cross Section Database.

The Atomic Spectra Database (ASD) [1] offers evaluated data on energy levels, wavelengths, and transition probabilities for atoms and atomic ions. Data are given for some 950 spectra and 70,000 energy levels. About 91,000 spectral lines are included, with transition probabilities for about half of these. Additional data resulting from our ongoing critical compilations will be included in successive new versions of ASD. We plan to include, for example, our recently published data for some 16,000 transitions covering most ions of the iron-group elements, as well as Cu, Kr, and Mo [2]. Our compilations benefit greatly from experimental and theoretical atomic-data research being carried out in the NIST Atomic Physics Division. A new compilation covering spectra of the rare gases in all stages of ionization, for example, revealed a need for improved data in the infrared. We have thus measured these needed data with our high-resolution Fourier transform spectrometer [3].

An upcoming new database will give wavelengths and intensities for the stronger lines of all neutral and singly-ionized atoms, along with energy levels and transition probabilities for the persistent lines [4].

A critical compilation of the transition probabilities of Ba I and Ba II [5] has been completed and several other compilations of atomic transition probabilities are nearing completion. These include data for all spectra of Na, Mg, Al, and Si [6]. Newly compiled data for selected ions of Ne, Mg, Si and S, will form the basis for a new database intended to assist interpretation of soft x-ray astronomical spectra, such as from the Chandra X-ray Observatory. These data will be available soon on the World Wide Web [7].

References:

- 1. D. E. Kelleher, et al., Atomic Spectra Database, Ver. 2.0, (http://physics.nist.gov/asd).
- 2. T. Shirai, et al., Spectral Data for Highly Ionized Atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo, J. Phys. Chem. Ref. Data, Monograph 8, (2000).
- 3. C. J. Sansonetti, et al., to be published.
- 4. J. E. Sansonetti, W. C. Martin, Handbook of Basic Atomic Spectroscopic Data, in press (2002).
- 5. J. Z. Klose, et al., J. Phys. Chem. Ref. Data, in press (2002).
- 6. D. E. Kelleher, L. I. Podobedova, to be published.
- 7. L. I. Podobedova, et al., Spectral Data for the Chandra X-ray Observatory, in preparation.