Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities

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All modern concepts of implementation of thermonuclear fusion for energy production involve high-temperature plasmas confined by different methods. These plasmas generally contain impurities of multiple chemical elements in various stages of ionization. These impurities can be used to control and diagnose the plasma conditions. In both cases, extensive kinetic modeling is required in order to produce a predictable response of plasma parameters to changes in impurity contents and extract the plasma parameters from observed spectra. This implies that a large quantity of atomic data must be precisely known. One of the primary goals of the Atomic Spectroscopy Data Center of the National Institute of Standards and Technology (NIST) is to provide such critically evaluated data to the fusion research community. I will describe the methods we are using in this compilation process. Our procedure begins with an exhaustive review of the literature for relevant data. This process makes use of our online bibliographic databases. The critical assessment of atomic wavelengths and their energy-level classifications is based on level schemes and theoretical interpretations that have survived examinations for consistency (experimental, isoelectronic, theoretical). Reliable line classifications are thus a primary output of our evaluations of the laboratory data and analysis. We include leading eigenvector percentages for the energy levels, where available, and references to theoretical calculations in our level compilations. These give an immediate indication whether large deviations from, for example, Russell-Saunders multiplet intensities can be expected and serve as a guide to the theoretical literature. Calculations are used to help discriminate between possible contradictory line classifications. Our critical assessment of atomic transition probabilities follows a well-developed systematic approach. This is a key element of our work, since practically all calculated data – the great majority of our available transition probability data – do not include uncertainty estimates. In our approach, a uniform critical assessment of the data provides the basis for data selection and assignment of numerical uncertainties. All data are reviewed with respect to the following four primary criteria: 1) the author's evaluation and numerical estimate of the uncertainties, 2) the degree of agreement of the results with other reliable data, 3) the author's consideration of critical factors (such as cascading in lifetime experiments or self-absorption in emission experiments) affecting the results, and 4) the degree of fit of the results into established systematic trends, or the reasons for possible deviations. In special cases, additional criteria may be used, such as comparisons of calculated and observed relative intensities of spectral lines. On the basis of this assessment the most reliable data are selected. Finally, the data are characterized with respect to their uncertainties on a scale from AA (less than 1%) to E (greater than 50%). A detailed description of our assessment procedure is given in Wiese et al. J. Phys.Chem. Ref. Data Mon. 7 (1996).