J. Plasma Fusion Res. SERIES, Vol.7 (2006) 327-330

Critical Compilation of Wavelengths and Energy Levels for Atoms and Atomic Ions

READER Joseph

National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

(Received: 5 Octorber 2004 / Accepted: 20 May 2005)

Abstract

Current projects to critically compile wavelengths and energy levels for atoms and atomic ions at the National Institute of Standards and Technology are summarized.

Keywords:

atom, atomic ion, energy level, ionization energy, percentage composition, transition probability, wavelength

1. Introduction

At the National Institute of Standards and Technology (NIST) we are carrying out a systematic program of critical compilation of wavelengths and energy levels of atoms and atomic ions. The spectra to be compiled are selected according to their general importance to science and industry. For example, spectra of tungsten are expected to be important for diagnosing plasmas in next generation tokamak devices. Hence, we are now compiling the spectra and energy levels for W in all stages of ionization [1]. Similarly, the spectra of neon and argon are important for understanding many stellar objects as well as for diagnosing tokamak plasmas and we are thus in the process of compiling the spectra of all Ne and Ar ions, including the neutral atoms. The spectra of xenon are currently of great interest for planned extreme ultraviolet microlithography; we have just completed a comprehensive compilation of Xe in all stages of ionization.

For the most part, the data are experimental values based on laboratory observations. In some cases, such as for H-like and He-like ions, the data are derived from calculations with sophisticated atomic structure codes that include relativistic and quantum electrodynamic effects.

The process of producing a critical compilation requires the retrieval of all data from the literature for a particular ion. In many cases this may require that data be extracted from more than one paper. For neutral and singly-ionized atoms it is not uncommon for 10 or more papers to be used. Often the data from different papers are inconsistent and possibly contradictory. Where possible, we attempt to resolve these conflicts by use of isoelectronic comparisons and ab initio calculations. In some cases level identifications given in the literature are incomplete in their specifications, and new calculations are needed to obtain appropriate names. If available, we tabulate the percentage compositions for the observed levels. In many cases these compositions are taken from our own calculations.

When data from two or more papers are blended together to form a single list of lines and levels, it is usually necessary to derive a new set of levels and to optimize their values so that the differences of the level values (Ritz values) best reproduce the observed spectrum. This is usually done with a computer code [2] that weights the wave numbers according to their uncertainties and minimizes the differences between the observed wave numbers and those derived from the levels in an iterative procedure. The final Ritz wavelengths are generally more accurate than those that were observed.

Finally, it is often necessary for us to determine an ionization energy from the observed data. The accompanying paper [1] in this Conference by A.E. Kramida describes one method that we have developed for this purpose as well as other aspects of the compilation process. It also describes a new computer code for optimizing the energy level values.

In Fig. 1 we illustrate schematically the process of critically compiling wavelength and energy level data. As can be seen, our independent calculations play an important role in nearly all aspects of the process. The example is for a case where three literature sources are being consulted. Although in practice there may be only a single source that is needed, in many cases there may be many more that have to be blended together to form

Corresponding author's e-mail: joseph.reader@nist.gov

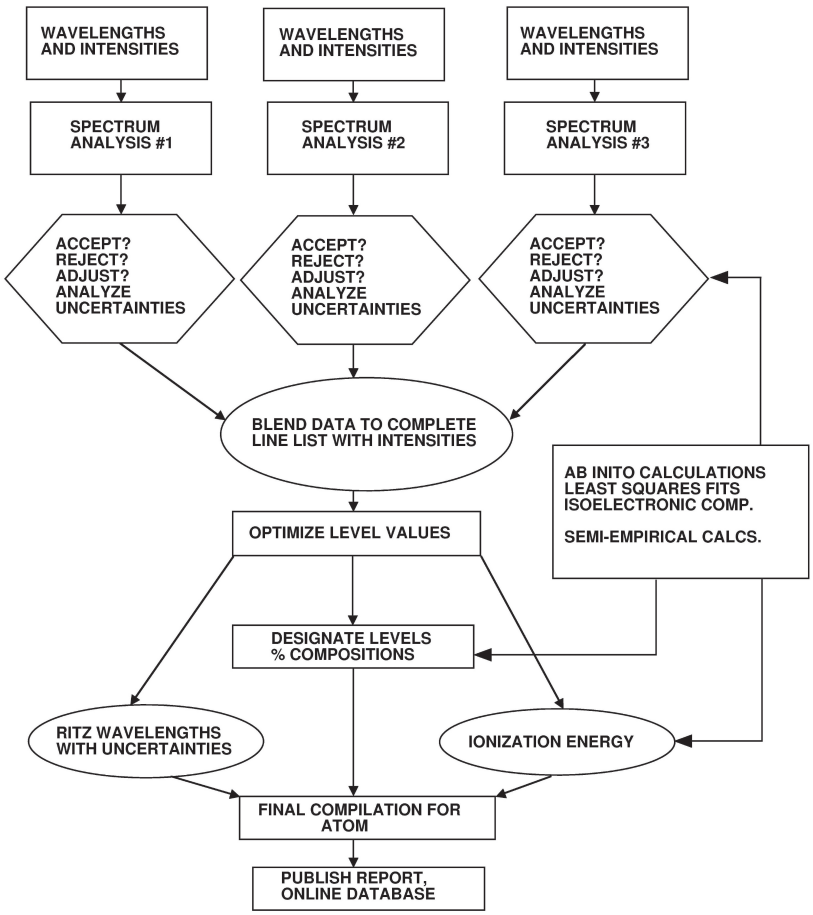

Fig. 1 Process of critical compilation of wavelength and energy level data.

the final compilation.

2. Current critical compilations of spectral lines and energy levels at NIST

We summarize our current projects:

2.1 E.B. Saloman, " Energy Levels and Observed Spectral Lines of Xenon, Xe I through Xe LIV, " J. Phys. Chem. Ref. Data 33, 765-921 (2004).

The energy levels and observed spectral lines of the xenon atom, in all stages of ionization for which experimental data are available, have been compiled. Sufficient data were found to generate level and line tables for Xe I-Xe XI, Xe XIX, Xe XXV-Xe XXIX, Xe XLIII-Xe XLV and Xe LI-Xe LIV. For Xe LIII and Xe LIV theoretical values are compiled for the energy levels. In 15 of the other stages a few lines are reported. Experimental g-factors are included for Xe I, Xe II and Xe III. A value, either experimental, semiempirical, or theoretical, is included for the ionization energy of each ion.

2.2 E.B. Saloman and C.J. Sansonetti, "Wavelengths, Energy Level Classifications and Energy Levels for the Spectrum of Neutral Neon, J. Phys. Chem. Ref. Data in press (2004).

We have prepared a comprehensive critically evaluated compilation of the most accurate wavelength measurements for classified lines of neutral neon (Ne I) in its natural isotopic abundance. Data from 19 sources spanning the region 256 Å to 54 931 Å are included. Based on this line list we have derived optimized values for the energy levels of neutral neon. Tabular data for 1595 classified lines and 374 energy levels are provided. In addition to the observed wavelengths, we present revised wavelengths calculated from the optimized energy levels for all lines that have been previously recommended for use as secondary wavelength standards.

2.3 A.E. Kramida, " Critical Compilation of the Wavelengths and Energy Levels of Singly Ionized Beryllium (Be II), " Physica Scripta in press (2004).

Energy levels and wavelengths of the second spectrum of beryllium (Be II) were critically compiled. Energies of the levels involving excitation of the valence electron were re-optimized using the new data on tran-

sition wavelengths or calculated using precise semi-empirical formulas. Energies of the doubly- and triply-excited terms were taken from a recently published compilation [A.E. Kramida, Physica Scripta **57**, 66 (1998)] or obtained from recently published Auger electron spectra. Observed wavelengths and wavelengths calculated from the differences of the upper and lower levels are given together with their uncertainties.

2.4 A.E. Kramida, " Critical Compilation of Wavelengths, Energy Levels and Transition Probabilities for W I and W II, " J. Phys. Chem. Ref. Data submitted (2004).

Energy levels, wavelengths and transition probabilities of the first and second spectra of tungsten, W I and W II, have been compiled. Wavelengths of observed transitions and energy levels derived from those wavelengths have been obtained from a critical evaluation of the available literature. Measured transition probabilities for some of the observed transitions have been compiled from the published literature.

2.5 J.J. Curry, " A Critical Compilation of Wavelengths, Energy Levels and Transition Probabilities for Ba I and II, " J. Phys. Chem. Ref. Data 33, 725-746 (2004).

Energy levels, wavelengths, and transition probabilities for the first and second spectra of barium, Ba I and Ba II, have been compiled. Wavelengths of observed transitions and energy levels derived from those wavelengths have been obtained from a critical evaluation of the available literature. Measured and calculated transition probabilities for some of the observed transitions have been obtained from the recent compilation of Klose, Fuhr and Wiese (J. Phys. Chem. Ref. Data **31**, 217 (2002)).

2.6 W.Whaling, W.H. C. Anderson, M.T. Carle, J.W. Brault and H.A. Zarem, " Argon I Lines Produced in a Hollow Cathode Source, 332 nm -5865 nm, " J. Res. Natl. Inst. Stand. Technol. 107, 149-169 (2002).

We report precision measurements by Fourier transform spectroscopy of the vacuum wave number, line width and relative signal strength of 928 lines in the Ar I spectrum. Wavelength in air and classification of the transition are supplied for each line. A comparison of our results with other precision measurements illustrates the sensitivity of Ar I wavelengths to conditions in the light source.

2.7 J.E. Sansonetti, " Wavelengths, Transition Probabilities and Energy Levels for the Spectra of Rubidium (Rb I through Rb XXXVII), " J. Phys. Chem. Ref. Data to be submitted.

Energy levels, with designations and uncertainties, have been compiled for the spectra of the neutral atom and all positive ions of rubidium ($Z = 37$). Wavelengths with classifications, intensities, and transition probabilities are also tabulated. In addition, ground states and ionization energies are listed. For most ionization stages experimental data are available; however for ionization stages where only theoretical calculations or fitted values exist, these are reported. There are a few ionization stages for which only a calculated ionization energy is available.

2.8 A.E. Kramida and G. Nave, " Optimized energy levels, level naming, new FTS measurements and compiled spectral lines of Ne II, " Eur. Phys. J. D to be submitted.

Spectra of neon-filled hollow cathode discharge lamps were observed by means of high-resolution Fourier-transform spectroscopy (FTS) covering the region from vacuum ultraviolet to near infrared. Combining these new measurements with results of other FTS and conventional-spectroscopy observations, we compiled a complete list of approximately 1700 spectral lines of Ne II covering the range from 324 Å to 13 μm. All known energy levels of Ne II were derived from this line list with improved accuracy. The newly optimized energy levels were used to derive a set of Ritz wavelength standards in the vacuum ultraviolet that are in good agreement with previously used data. With the help of parametric calculations, an improved classification of energy levels was made and the existing controversy in the naming of strongly mixed levels was resolved.

2.9 A.E. Kramida and G. Nave, " New FTS measurements, optimized energy levels and refined VUV standards in the Ne III spectrum, " Eur. Phys. J. D to be submitted.

All observed spectral lines of Ne III in the range 204 Å to 36 μm have been compiled and critically evaluated. Fifty seven visible and ultraviolet lines of Ne III have been precisely measured using Fourier transform spectroscopy. An optimized level scheme has been derived from the total list of observed lines. Relative positions of about 180 out of a total of 226 previously known energy levels of Ne III have been determined with improved accuracy compared to previous studies. Excitation energies of almost all levels have been re-

vised by 1.5 to 2.0 cm^{-1}. More than 100 precise wavelength standards in the region 210 to 2900 Å with well-defined uncertainties have been derived. Concepts of error current and covariance matrix have been implemented in a computational algorithm that permits one to derive the uncertainties of Ritz wavelength standards obtained from a set of least-squares-optimized energy levels. Nine new energy levels have been found and 16 new transitions have been identified in the extreme ultraviolet region. The ionization potential has been increased by 4.5 cm^{-1}. The new value is 511543.5 ± 2.7 cm^{-1}(63.4233 ± 0.0003 eV).

3. Compilations in progress at NIST

The following compilations are currently in progress:

1. Wavelengths and energy levels for Kr in all stages of ionization (E.B. Saloman).
2. Wavelengths and energy levels for Ga in all stages of ionization (T. Shirai, J. Reader, A.E. Kramida and J. Sugar).
3. Wavelengths and energy levels for Sr in all stages of ionization (G. Nave).
4. Wavelengths and energy levels for Ba III- Ba LVI (J.J. Curry).
5. Wavelengths and energy levels for Ar in all stages of ionization (C.J. Sansonetti and T. Shirai).
6. Wavelengths and energy levels for W III-W LXXVI (T. Shirai and A.E. Kramida).
7. Wavelengths, energy levels, and transition probabilities for Cs in all stages of ionization (J.E. Sansonetti).
8. Wavelengths and energy levels for Ne VII and Ne VIII (A.E. Kramida).

This work is supported in part by the Office of Fusion Energy Sciences of the U.S. Department of Energy and by the U.S. National Aeronautics and Space Administration.

References

[1] A.E. Kramida, paper P2-61, this Conference.

[2] For this purpose, we often use the program ELCALC, written by L.J. Radziemski (The Research Corporation, Tucson, Arizona, 85712, U.S.A.) The procedure and definition of level value uncertainties are described in L.J. Radziemski, Jr. and V. Kaufman, J. Opt. Soc. Am. **59**, 424 (1969). A more advanced code for this purpose, LOPT, has been written by A.E. Kramida, see reference [1].