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Critically Assessed Tables of Atomic Spectroscopy Data

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Abstract: The major NIST atomic spectroscopy data tables and the new NIST atomic spectra database (ASD) on the Internet are briefly reviewed. The need for critical assessments of atomic transition probability data is discussed, and the still unsatisfactory data situation for N II is presented as an example.

1. Introduction

The principal quantities characterizing atomic spectra are:

Wavelengths,
Energy levels and Ionization Potentials,
and Atomic Transition Probabilities (Oscillator Strengths).

At the National Institute of Standards and Technology (NIST), formerly the National Bureau of Standards (NBS), two data centers are operated to critically evaluate and compile numerical reference data for these quantities. The data compilation activities have been pursued for several decades, starting with the 1949 tables of "Atomic Energy Levels" by C. E. Moore [1].

In the last 20 years, the following major tables have been published by the NIST data centers in book form:

- Atomic Energy Levels of the Rare Earth Elements (1978 [2]).
- Wavelengths and Transition Probabilities for Atoms and Atomic Ions (covering the first through fifth spectra of all elements) (1980, 1997 [3-5]).
- Atomic Energy Levels of the Iron Period Elements- Potassium through Nickel (1985, [6]).
- Atomic Transition Probabilities-Scandium through Manganese, and Iron through Nickel (1988, [7,8]).
- Tables of Spectra of Hydrogen, Carbon, Nitrogen and Oxygen Atoms and Ions (1993, [9]).

- Atomic Transition Probabilities of Carbon, Nitrogen and Oxygen (1996, [10]).

2. The new comprehensive NIST database on the Internet

The material from all these volumes as well as additional critically evaluated data from recent smaller compilations is be incorporated in a comprehensive, electronically accessible database that will shortly go up on the World Wide Web. A preliminary version (version 1) of this general database with the same structure, but with a much smaller data set, has been already operational for the last three years under the following URL listing

http://physics.nist.gov/asd

The new greatly expanded version 2, called the "NIST Atomic Spectra Database" (ASD is scheduled to be released in the spring of 1998, under the same URL.
The holdings of version 1 and 2 of this database with regard to energy levels, wavelengths and transition probabilities are shown in Figure 1, 2 and 3 for the various chemical elements (in order of atomic numbers) and stages of ionization (in order of charge states, from neutral (0) to the most highly charged ion). In total, ASD contains data for about 950 spectra, with about 70000 energy levels, 85000 line wavelengths and about 40000 transition probabilities.

The data are displayed in formats similar to those in the NIST printed spectroscopic data tables. The two principal categories of queries handled by the database are for data on energy levels and for data on spectral lines. Many different search options and selections are available to the user. For example, a limited wavelength range may be specified, the number of species may be limited, and transitions may be arranged by multiplets as well as in order of wavelengths.

3. The need for critical evaluations

Spectroscopic data are determined by a fairly large variety of experimental and theoretical approaches, and these have become increasingly sophisticated and complex, capable of ever increasing accuracy. The accuracy reached in laboratory determinations for the wavelengths of spectral lines, as well as for the related energy levels derived via the Ritz combination principle, is normally better than needed for the majority of applications. Thus, normally no problems arise with respect to the accuracy of these spectroscopic data. But for atomic transition probabilities or oscillator strengths, the situation is quite different.

The large majority of the data comes from sophisticated calculations. No unambiguous uncertainty estimates are possible for these results because of the many approximations that are involved. But numerous substantial differences exist, even between the results of the most advanced calculations, especially for weaker transitions. On the other hand, experimental oscillator strength data, which allow realistic estimates of uncertainties, are comparatively sparse. But even for these, a fair number of discrepancies, sometimes far outside the mutually estimated uncertainties, have been encountered between different experiments.

For the tabulation of reference data it is therefore of crucial importance that transition probabilities are critically assessed and that in cases where several results are available for the

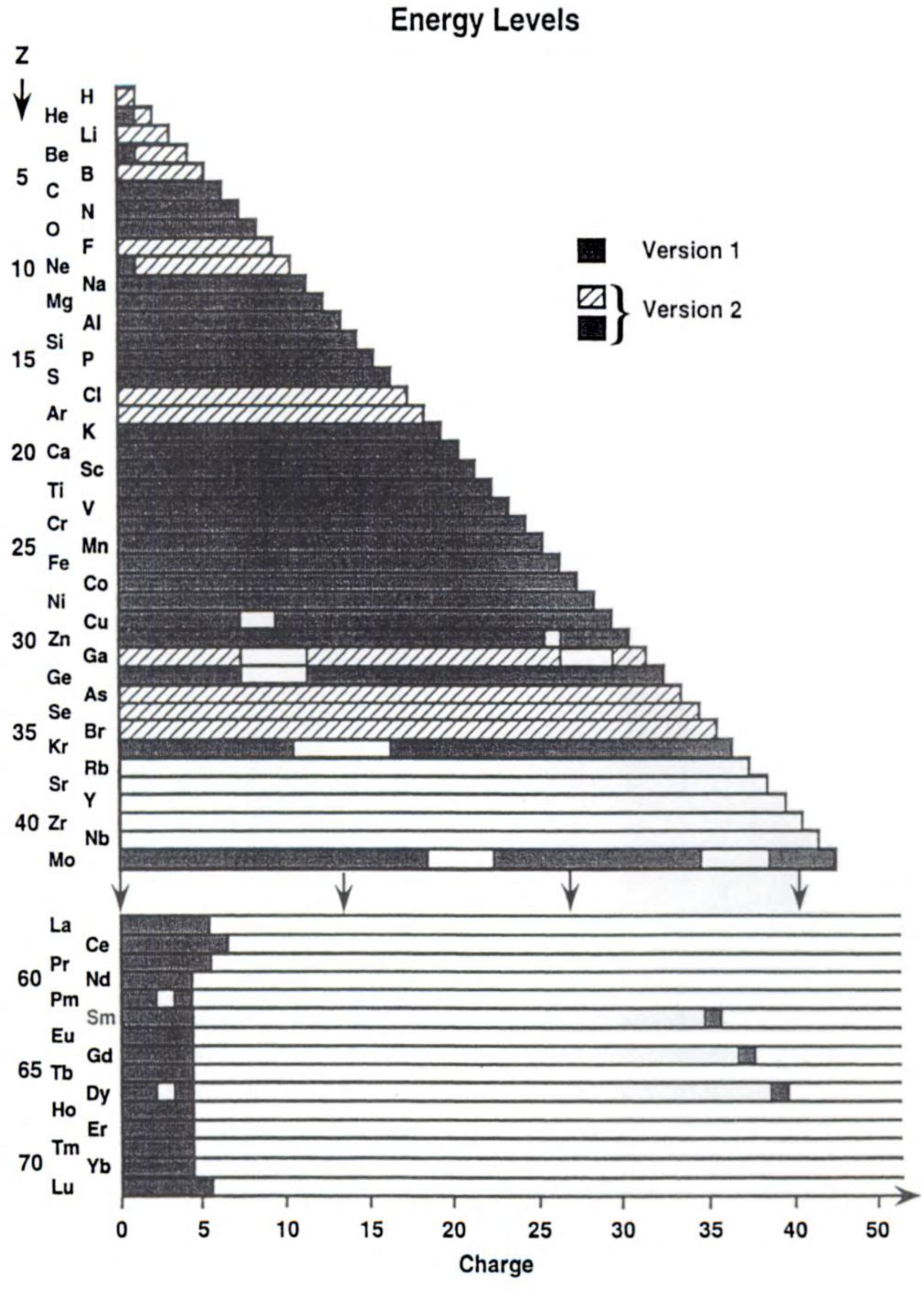

Figure 1: Holdings of energy-level data in Versions 1 and 2 of the NIST Atomic Spectra Database.

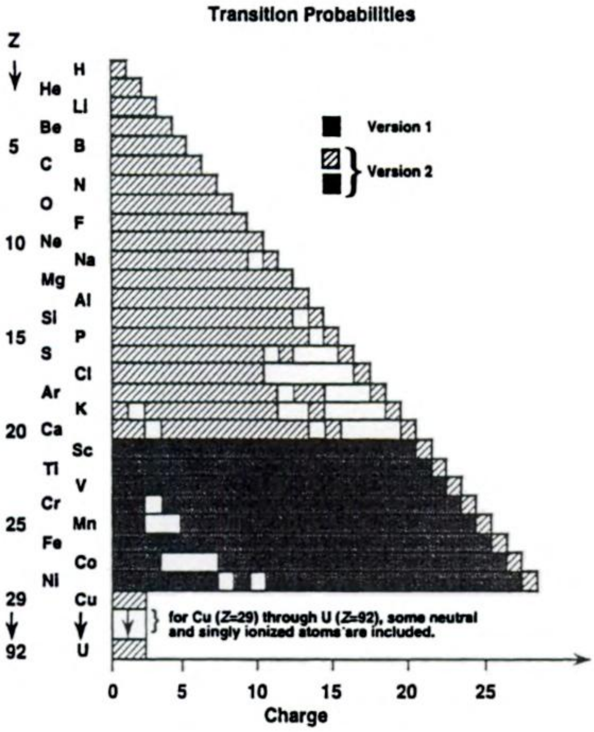

Figure 2: Holdings of transition-probability data in Versions 1 and 2 of the NIST Atomic Spectra Database.

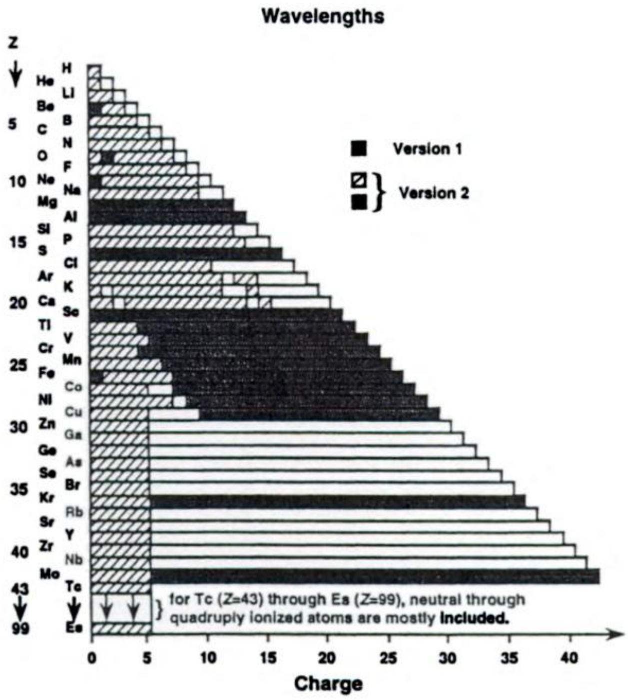

Figure 3: Holdings of wavelength data in Versions 1 and 2 of the NIST Atomic Spectra Database.

same transition, the best data are established through an assessment process. At NIST, we have therefore developed and refined such a procedure over the course of many years.

4. The assessment procedure for atomic transition probabilities

The NIST procedure is based on the following four general assessment criteria, to which each paper is subjected:

1. Consideration of the "critical factors" of a method by the authors.
2. The authors' estimates of the uncertainties of their measured (or calculated) data. (As noted above, in sophisticated calculations the uncertainties usually cannot be reliably tracked. Thus, estimates of uncertainties have been only made by comparisons with experiments.)
3. The degree of agreement with other reliable data, utilizing tabular or graphical comparisons.
4. The fit of the data into systematic trends, or deviations from them.

The "critical factors," which are specific to each method, have been discussed in detail before [10, 11], so that I will not review them here. Instead, a specific example may serve to illustrate the critical assessment process, and it will show as well the considerable uncertainties still encountered even in the transition probability data from advanced sources.

My example is the data situation for N II. For this spectrum (as well as for most other spectra of the lighter elements), a large amount of multiplet data (in this case 160 out of 256 multiplets recently tabulated by the NIST group [10]) has been produced by the "Opacity Team" [12,13]. All data are calculated with a modified close-coupling approach in conjunction with the R-matrix method. The wavefunctions for the target ion—in this case N III—are constructed with the configuration interaction code CIV 3, and the full atomic system, with the "captured" electron added, is described by the close coupling approach.

Another sophisticated and rather extensive calculation has been performed by Bell et al. [14], who have used the configuration interaction code CIV 3 directly to determine the wavefunctions of various excited states of N II. Fig.4 shows a comparison of the Opacity Project [13] and the Bell et al. [14] results for all multiplets where they overlap. The comparison shows excellent agreement for the multiplets with large line strengths S (or large oscillator strengths), but the scatter increases sharply as the line strengths become smaller. In addition, some high quality experimental data as well as results from other advanced calculations are available for N II (for detailed literature citations of all of these, see ref. [10]).

Unfortunately, all of these data concern the stronger lines only and do not provide any insight into the course of the discrepancies for the weaker lines and multiplets. A similar situation is encountered for many other spectra of light elements: When data from both the Opacity Project calculations and the fundamentally different CIV 3 configuration interaction calculations are available on a fairly extensive basis, the results are typically in

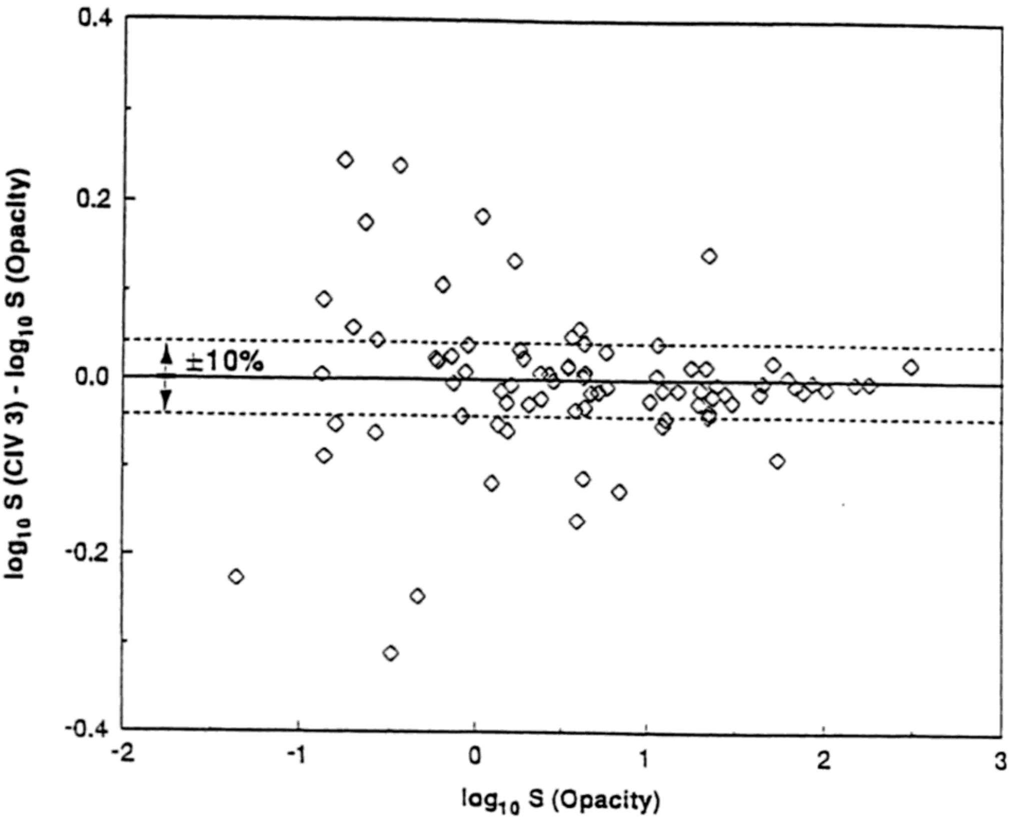

Fig.4. Comparison of the OP multiplet data by Luo and Pradhan [13] with the results of the CIV 3 calculations by Bell et al. [14]. The OP/CIV 3 multiplet ratios are plotted on a logarithmic scale versus log S of the OP data. The broken lines indicate a band of deviations of ± 10% around a perfect ratio of 1.00. The figure shows that the scatter in the ratios increases significantly for the weaker multiplets.

excellent agreement for most strong multiplets, i.e., they agree within a few percent, but they differ a great deal for the weaker multiplets, and this appears to be pretty much a random pattern.

The relevant "critical factors" for advanced calculations are:

- extensive configuration interaction treatments
- good agreement of the dipole length and dipole velocity forms
- convergence to the final result as the number of configurations increases
- close match of calculated and experimental transition energies

Indeed, many oscillator strengths for the light elements have been calculated both with the dipole length and velocity forms, and it is seen that for many weaker transitions the

the dipole length and velocity forms, and it is seen that for many weaker transitions the differences are substantial. Also, the calculated transition energies are often checked against the experimental data. On the other hand, very few convergence studies have been done. Thus, the critical factors are either not satisfied for the weaker transition or are not fully addressed, and the present situation is clearly not satisfactory yet. Further progress is only likely to be achieved if either the critical factors are adequately satisfied or if a good number of high quality experimental comparison data should become available and would consistently support one of the calculations.

5. Conclusions

In conclusion, the representative example discussed above shows that critical assessments of atomic transition probabilities are essential in order to obtain realistic estimates of their often still sizable uncertainties. The NIST assessment procedure has been developed to address the uncertainty problem in an objective, consistent manner.

References

[1] Moore C E 1949 *Atomic Energy Levels* NBS Circular 467 (reprinted as Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 35 (1971))

[2] Martin W C, Zalubas R and Hagan L 1978 *Atomic Energy Levels — The Rare-Earth Elements* (Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.)60)

[3] Reader J, Corliss C H, Wiese W L and Martin G A 1980 *Wavelengths and Transition Probabilities for Atoms and Atomic Ions* (Natl. Stand. Ref. Data Ser., Natl. Bur. Stand (U.S.)68)

[4] Reader J and Corliss C H (Eds.) 1997 *Line Spectra of the Elements*, in CRC Handbook of Chemistry and Physics 78th Edition (Boca Raton: CRC Press)

[5] Fuhr J R and Wiese W L 1997 *NIST Atomic Transition Probability Tables*, in CRC Handbook of Chemistry and Physics, 78th Edition (Boca Raton: CRC Press)

[6] Sugar J and Corliss C H *Atomic Energy Levels of the Iron Period Elements: Potassium through Nickel J. Phys. Chem. Ref. Data* **14,** Supplement No. 2

[7] Martin G A, Fuhr J R and Wiese W L 1988 *Atomic Transition Probabilities-Scandium through Manganese J. Phys. Chem. Ref. Data* **17**, Supplement No. 3

[8] Fuhr J R, Martin G A and Wiese W L 1988 *Atomic Transition Probabilities-Iron through Nickel J. Phys. Chem. Ref. Data* **17,** Supplement No. 4

[9] Moore C E 1993 *Tables of Spectra of Hydrogen, Carbon, Nitrogen and Oxygen Atoms and Ions* (J. W. Gallagher, Editor, Boca Raton: CRC Press)

[10] Wiese W L, Fuhr J R and Deters T M 1996 *Atomic Transition Probabilities of Carbon, Nitrogen and Oxygen J. Phys. Chem. Ref. Data* Monograph No. 7

[11] Wiese W L 1996 *Phys. Scr.* **T65**, 188-191

[12] The Opacity Project Team 1995 *The Opacity Project*-Vol. I (Bristol IOPP)

[13] Luo D and Pradhan A K 1989 *J. Phys. B* **22**, 3377

[14] Bell K L, Hibbert A and Stafford R P 1995 *Phys. Scr.* **52**, 240.