RECENT DEVELOPMENTS IN ATOMIC TRANSITION PROBABILITIES

W. L. Wiese
National Bureau of Standards
Washington, D.C. 20234 U.S.A

In the last decade, research to determine atomic transition probabilities has proceded at a steady pace. Currently, the main needs for transition-probability data arise from astrophysics, magnetic fusion-energy research, and laser development. The principal approaches for the determination of data have undergone further refinement and the major conventional techniques generally contribute data in roughly the same proportions as earlier. However, some significant changes have also occurred: theoretical approaches, especially semi-empirical approximations, have produced vastly increased amounts of data; on the experimental side, determinations of atomic lifetimes by beam-foil spectroscopy have shown a decline, but work utilizing the branching-ratio emission technique as well as lifetime techniques involving laser excitation are on the increase.

Atomic transition probability or oscillator strength (f-value) data have been notorious for their rather low accuracy, especially when compared to other spectroscopic data. For example, of the 5000 allowed lines contained in the 1969 NBS data tables for the elements sodium through calcium (Z=11-20)[1], only two lines -the sodium resonance doublet -were rated with an accuracy better than 3 percent, while most other lines in this book are estimated to be in the 25 to 50 percent accuracy range. During the last decade, significant progress has been made in improving the accuracy of transition-probability data. The most advanced theoretical approaches have come up with more reliable data by including configuration mixing on a larger scale as well as by accounting for core-polarization effects. For fairly simple atomic systems the results are usually in the 10-percent accuracy range, as many comparisons with the best experimental data have shown. In addition, for some transitions of helium[2], lithium[3], beryllium[4] and some ions of their isoelectronic sequences, a recently developed technique of calculating rigorous upper and lower error bounds for transition probabilities, introduced by Weinhold[5], has been able to provide theoretical error limits for the first time; these are quite narrow for some of the transitions treated. On the experimental side, impressive progress has been made, too, especially with lifetime studies. The most accurate lifetime data have probably been determined by Andrae and co-workers.[6] For example, Gaupp[7] of this group has recently determined lifetime and transition-probability data for the resonance transitions of lithium and sodium with a probable error of two-tenths of a percent, which probably represents the current experimental record for the most accurate transition probabilities. Significantly, however, each of the two measured f-values is distinctly lower than all the best theoretical data, but within the rigorous theoretical error bounds. An extensive series of high-precision measurements has been made by Blackwell and co-workers[8] for the relative absorption oscillator strengths of several hundred lines of Fe I and Ti I and II. These data have been determined with an accuracy of about one percent or better, and the Fe I data have been converted to almost equally

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accurate absolute values by using very accurate lifetime data for the principal resonance line of Fe I at 3720 Å. Improvements in the accuracy of emission and hook techniques have been very significant, too. As a few examples, one might mention the precise Ar I emission experiments by Nubbemeyer[9] in 1976 and Preston[10] in 1977, obtained with stabilized high-current arc sources, which yielded absolute transition probabilities with probable errors on the order of 5 and 7 percent, respectively. Also noteworthy are the accurate hook, emission, absorption, and branching-ratio emission measurements by Huber, Kock, Whaling, and others (see, e.g., Refs. 11-13) that have produced data in the 10-percent range.

The increased accuracy has been obtained through significant advances in instrumentation as well as refinements in the measurement methods and in the plasma models applied. In most cases, this has at the same time meant increased complexity, and thus more effort, to obtain relatively few data. Thus, a general drawback of precision measurements is that they are more time consuming than much of the earlier work. At the current rate of output, such efforts will make significant improvements in the data base only over a period of many years.

Since needs for large sets of data are as urgent as ever, especially for astrophysical studies, some theoretical work has been under way to satisfy these needs with techniques where some accuracy is sacrificed in order to be able to obtain large quantities of data. One needs to mention here especially the very extensive semi-empirical calculations by Kurucz and Peytremann[14], because of their enormous astrophysical importance. These authors have calculated f-value data for about 2 million lines of the lower ions of iron-group elements. Kurucz's most recent work[15] concerned the spectrum of Fe II, where he was able to utilize a much improved and extended set of experimentally determined energy levels for the fitting of his computed eigenvalues. In this case he obtained fairly good agreement with the existing experimental f-value data, while in the earlier work larger differences with experimental results occurred -seemingly at random. Comparisons between Kurucz's calculated data and the best experimental data quoted in the NBS critical compilations (discussed below) are shown for two sample cases in Figs. 1 and 2.

Another significant large-scale contribution is the recent work by Gurtovenko and Kostik[16], who have determined about 1000 lines of Fe I from solar spectral data

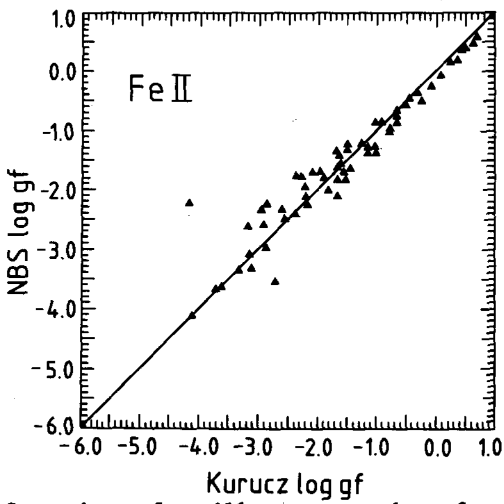

Fig. 1: Comparison of oscillator strength or f-value data (multiplied by the statistical weight g of the lower state) calculated semi-empirically by Kurucz[15] versus experimental data critically selected for the recent NBS tabulation[22], which are estimated to have uncertainties within ±50%.

in conjunction with recent solar models. A significant part of their data overlaps with laboratory results. The agreement is excellent for weaker and moderately strong lines, of log gf < -1.0 (g is the statistical weight of the lower state), but becomes systematically worse for stronger lines, as shown in Fig. 3.

The above sampling of recent work represents, of course, only a very small part of the total effort in this field and the selection of references has been rather arbitrary. For a complete listing of all recent experimental and theoretical work on atomic transition probabilities, the NBS bibliographies[17] as well as the special new bibliography prepared for the report of Working Group 2 of Commission 14 of the IAU should be consulted.[18]

The collection of the atomic-transition-probability literature as well as comprehensive critical compilations of numerical data are carried out at the U.S. National Bureau of Standards. A small data-evaluation group has been in existence there for 20 years. During the last 10 years, the work of this group has concentrated on the critical compilation of f-value data for the elements of the iron group -i.e., Sc, Ti, V, Cr, Mn, Fe, Co, and Ni -in all stages of ionization, which amounts to a total of about 190 spectra. Numerical data for approximately 10,000 allowed and forbidden lines have been critically evaluated and tabulated. Four separate compilations[19-22] -for Sc and Ti[20]; for V, Cr, and Mn[21]; for Fe, Co, and Ni[22]; and for the forbidden lines[19] -have already been published and all these tables are presently being updated, with many newly available data added. It is planned to republish all these spectra within the next year as the third volume of the NBS data series. Also this center has recently published a table of transition probabilities for 5000 selected lines of many elements[26]. A list of the principal data output of the NBS center is given in Table 1. The NBS data center also

Table 1

NBS Compilations of Atomic Transition Probabilities

Atomic Number Z	Elements	Book or Journal	Reference
1-10	H, He, Li, Be, B, C, N, O, F, Ne	NSRDS-NBS 4 (Vol. I)	23
11-20	Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca	NSRDS-NBS 22 (Vol. II)	1
21,22	Sc, Ti	J. Phys. Chem. Ref. Data	20
23-25	V, Cr, Mn	J. Phys. Chem. Ref. Data	21
26-28	Fe, Co, Ni	J. Phys. Chem. Ref. Data	22
23-28	Forbidden lines V-Ni	J. Phys. Chem. Ref. Data	19
3-28	Ions of the Li isoelectronic sequence up to Ni XXVI	J. Phys. Chem. Ref. Data	24
56	Ba I and II	Atomic Data	25
1-92	5000 selected lines of many elements	NSRDS-NBS 68; and CRC Handbook of Chem. and Phys.	26

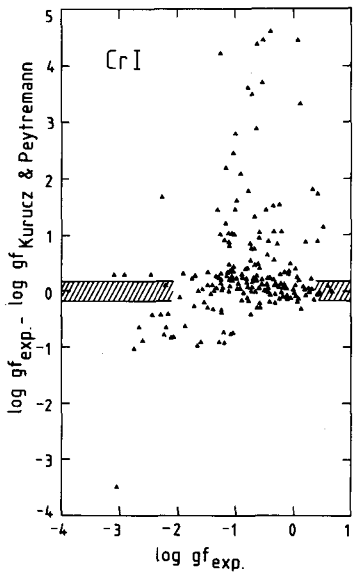

Fig. 2: Comparison of oscillator strength (or f-value data) calculated semi-empirically by Kurucz and Peytremann[14] for Cr I versus experimental data critically selected for the NBS table [21], which are estimated to have uncertainties within ±50%. The shaded band indicates the areas where the agreement between theory and experiment is within ±50% (Δlog gf < 0.17).

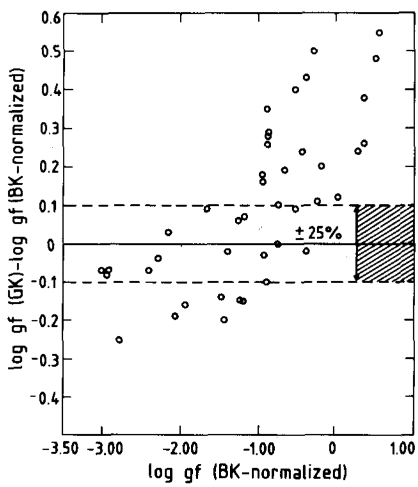

Fig. 3: Comparison of f-values obtained from solar data by Gurtovenko and Kostik[16] with the arc emission data by Bridges and Kornblith[27] (as normalized in the NBS tables by Fuhr et al.[22]), which are estimated to have uncertainties within ±25%. This as well as similar comparisons with other data tabulated in Ref. 22 show that the solar f-values derived by Gurtovenko and Kostik have a systematic tendency to overestimate the oscillator strengths of spectral lines for which log gf > -1.0.

continues to collect all f-values literature and will publish bibliographies from time to time. The latest supplement appeared in 1980.[17] The center is now in the process of automating its files of bibliographical material and critically evaluated numerical data so that in the not too distant future it should be possible to retrieve bibliographical and numerical data entries by computer. Aside from the data automation efforts at NBS, some other attempts to generate transition-probability data banks appear to be under way; however, detailed information on the output is not yet available.

The long-range goals of the NBS data center are: (a) to compile transition probabilities for selected heavy elements, especially those of interest to space astronomy and magnetic-fusion energy; and (b) to update and expand the transition-probability tables for the first ten elements, hydrogen through neon, which were published by NBS in 1966 and which are now out of date.

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