This Week's Citation Classic

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Wiese W L, Smith M W & Glennon B M. Atomic transition probabilities. Volume 1: hydrogen through neon. Washington, DC: US Government Printing Office, 1966. 153 p. NSRDS-NBS 4.

[Institute for Basic Standards, National Bureau of Standards, Washington, DC]

Atomic transition probabilities are the atomic quantities characterizing the strength of spectral lines. This compilation contains critically evaluated data for about 4,000 spectral lines of the lightest 10 elements, hydrogen through neon, and lists also other key spectroscopic data on these spectral transitions. [The SCI® indicates that volume 1 of this title has been cited in over 1,255 publications. All the volumes of this title have been cited in over 2,000 publications.]

A Critical Table of Atomic Transition Probabilities

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This book is the first of a set of four books in which atomic transition probabilities are critically evaluated and compiled. ¹⁻³ It represents the first comprehensive tabulation of these atomic data on a selected basis and thus provides reference values for such important chemical elements as hydrogen, helium, carbon, nitrogen, and oxygen.

Of central importance in such a compilation is the judgment of the accuracy of the data. We had anticipated that the uncertainties would be quite significant and found that about one-third of all tabulated data were no better than of ± 50 percent accuracy. We also judged that data with uncertainties of less than 3 percent existed only for transitions of hydrogen-like and helium-like species. The experimental papers normally contained uncertainty estimates by the authors, but no such estimates were given for results from theoretical atomic structure calculations since their complexity simply did not allow any reasonable tracking of errors. From extensive comparisons of literature data, we noticed that some authors seemed to be much too optimistic, i.e., their results disagreed with other work far outside the mutual error estimates. On the other hand, our comprehensive tabulation only became possible because many reliable values had appeared in the literature, and the majority of

independent results were in good agreement with each other, within their estimated uncertainties.

In order to facilitate the critical evaluation. we tried to find "critical factors" in the different approaches that would guide us in the determination of the quality of the data. We established a set of such critical factors for each major method1 that we then utilized in all following tables and that have been now also generally accepted by researchers. For example, in emission experiments, the critical factors are validity of the normally assumed local thermodynamic equilibrium, consideration of self-absorption effects, the quality of the diagnostic technique, the radiometric intensity calibrations, and the line intensity measurement technique. Guided by the authors' consideration-or nonconsideration-of these critical factors, we often were more conservative in our final error estimates than the authors. This was especially true for the cited first volume where some such critical factors were not yet widely considered. For example, in the technique of utilizing emission intensity measurements, the consideration of and, if necessary, a correction for self-absorption effects is a critical factor. If it is not considered, significant systematic errors might occur.

Soon after the publication of the book, we received a number of protests by authors that we had not used their uncertainty estimates, but increased them, or that their work was not considered properly. Therefore, we periodically returned to check our published data against new, significantly improved experiments or calculations. We recently compared about a tenth of the data in this book with new, more advanced data and found that in about 75 percent of the cases the new and our critically selected older values are within the combined estimated error limits. For about one-half of the remaining 25 percent, the new data are only slightly outside our estimated error limits. However, if we would have used the original error estimates of the authors, agreement would have only been obtained in about 40 percent of all cases. We therefore feel that our system of critical factors is strongly supported by these later comparisons, and we believe that our realistic uncertainty estimates are probably also one of the reasons for the continued popularity and the many citations to this book.

Wiese W L, Smith M W & Miles B M. Atomic transition probabilities. Volume 2: sodium through calcium. Washington. DC: US Government Printing Office, 1969. 268 p. NSRDS-NBS 22. (Cited 815 times.)

Martin G A Fuhr J R & Wiese W L. Atomic transition probabilities—scandium through manganese. (Whole issue.)
J. Phys. Chem. Ref. Data 17(Supp. 3), 1988. 512 p.

Fuhr J R, Martin G A & Wiese W L. Atomic transition probabilities—iron through nickel. (Whole issue.)
J. Phys. Chem. Ref. Data 17(Supp. 4), 1988, 493 p.