Atomic Energy Levels and Other Spectroscopic Data

The key advances in our understanding of atomic structure were made early in the 20th Century. Niels Bohr developed his revolutionary theory of the hydrogen atom in 1913, still largely on classical terms. Then, in the 1920s, the generalization to other atoms and ions came with the development of quantum mechanics, or wave mechanics, by Schroedinger, Heisenberg and others, after de Broglie postulated that all elementary particles also have wave properties. Important later generalizations and refinements were the relativistic extensions by Dirac, as well as quantum electrodynamics by Feynman, Schwinger, and others. Even before these developments took place, many highly precise spectroscopic data had been obtained experimentally, and these data could now be fully understood in terms of atomic structure and quantum numbers. Thus, laboratory and astrophysical spectra could for the first time be interpreted as specific classified transitions between energy levels of atoms or positive ions.

The three volumes of tables in the *Atomic Energy Levels* series cited here [1-3] represented a synthesis of the data derived from studies of atomic spectra in the first half of the century—studies which played a major role in the revolution in physics just described. The effort can be traced to an initiative of the National Research Council, which in 1924 created a Committee on Line Spectra of the Elements, with one of its main goals being to encourage work on the analysis of atomic spectra and to collect atomic structure data in a systematic manner. A first, still rather incomplete, tabulation was undertaken by Bacher and Goudsmit in 1932 with a book entitled *Atomic Energy States as Derived from the Analysis of Optical Spectra* [4]. In the following years, spectroscopic data were accumulated on a vast scale, especially for somewhat heavier atoms and ions, and in the middle 1940s, with the strong support of the Line Spectra Committee, NBS Director E. U. Condon agreed to undertake a new data compilation project at NBS, after Bacher and Goudsmit declined to update their book. Charlotte E. Moore, already an expert in the compilation of atomic spectra and author of the Princeton Observatory *Multiplet Tables of Astrophysical Interest* of 1933 and 1945 [5], accepted a position at NBS in 1945 to prepare a handbook of atomic energy levels. This project achieved a first milestone in 1949 with the publication of Volume I of *Atomic Energy Levels,* containing the spectra of hydrogen, (atomic number Z=1) through vanadium (Z=23), 309 pages strong [1]. In 1952, Volume II with the elements chromium (Z=24) through niobium (Z=42) followed [2], and in 1958 a third volume containing the spectra of molybdenum (Z=42) through actinium (Z=89) completed this series [3], also known as NBS Circular 467.

In all these tables, the principal data presented are the atomic energy levels (or "energy eigenstates") compiled from experimentally determined (published or unpublished) material. This was done for those stages of ionization for which reliable data existed. All data were critically compiled, which means that in cases where several experimental results were available, only the best value was selected after critical evaluation. In addition to the level values, the spectroscopic configuration and term assignment, the total angular momentum quantum number, and the ionization energy of the atom or ion were presented, and all this material was arranged in a highly organized, easily readable format.

The NBS/NIST critical tables on atomic energy levels, wavelengths, and transition probabilities are the preeminent resource for atomic spectroscopy data.

As laboratory and astrophysical studies of atomic spectra and their application for plasma diagnostics and modeling became increasingly sophisticated, another principal spectroscopic quantity characterizing the strength of spectral lines assumed critical importance. This atomic constant is known as the atomic transition probability, or oscillator strength, or line strength. But atomic transition probabilities are much more difficult to determine precisely, both experimentally and theoretically. In the 1930s to 1950s, they were determined only on a small scale, and the uncertainties were—except for hydrogen—often quite large. But the situation gradually improved, and upon the urging of several scientific communities, NBS started to compile critically atomic transition probability data. Two volumes of *Atomic Transition Probabilities* covering the first twenty elements, i.e., hydrogen (Z=1) through neon (Z=10) and sodium (Z=11) through calcium (Z=20) were published in 1966 and 1969 by W. L. Wiese and coworkers [6,7]. These books were structured in a manner similar to the energy level volumes and contained both the transition probabilities and the equivalent expressions of oscillator strength and line strength, since different user communities work with different quantities. Both experimental and theoretical sources of data were utilized. In contrast to the highly precise energy level and wavelength data, the uncertainties of many transition probabilities were still appreciable, larger by orders of magnitude than those for wavelength and energy level data. Also, the body of available data was much smaller. Uncertainties can be directly determined for the experimental data, but this is nearly impossible for calculated results. For many prominent transitions, the available data were redundant, but often disagreed with each other. Therefore, a system for judging the quality of transition probability data became essential, and discussions of the data selections were presented for each spectrum. To this day, a coding system for the uncertainties is applied, with letters A to D, where A-class data are estimated accurate within ±3 % and the lowest admissible class of reference data is D, with uncertainties estimated not to exceed ±50 %. Detailed numerical uncertainty estimates are still not realistic in many cases.

In toto, C. E. Moore's atomic energy level books covered 75 chemical elements and 485 spectra in different ionization states. They became an essential tool for atomic, plasma, and astro-physicists as well as spectrochemists. About 7000 copies of each book were sold, and the books were reprinted in 1971 as NSRDS-NBS 35. The books were featured by "Current Contents" as a citation classic in 1990 [8] after they were cited in more than 7900 publications. This number has since then steadily increased to about 13 000 citations.

Similarly, the tables of atomic transition probabilities became widely used and cited. A total of about 7000 copies were sold. They were featured as citation classics [9] in 1989 and have been cited about 4000 times. Almost from the beginning, the spectroscopic data compilation program drew support from the user communities because of the need for comprehensive data sources that were critically evaluated. NASA and the Department of Energy have been long-term supporters of the data program and are continuing to support it to this date. User communities also voiced their strong support and published resolutions and expressions of need for the NBS/NIST data compilations. Examples include several resolutions by the General Assemblies of the International Astronomical Union (IAU), the latest in 1976, that "the IAU highly values the activities of NBS in the critical compilation of atomic and molecular data, and considers these activities essential for the advancement of astronomy" [10]. The spectrochemical community devoted a special issue of their journal Spectrochimica Acta to their atomic data needs [11].

Numerous personal letters of support and gratitude of leading physicists and astrophysicists have been received over the years, among them letters from the Nobelists Niels Bohr, Linus Pauling, Isidor Rabi, Gerhard Herzberg, Alfred Kastler, and Arthur Schawlow. Schawlow noted in one of his letters that the NBS spectroscopic data tables were essential tools in the search for new laser materials and laser wavelengths.

The NBS/NIST data program has been, and continues to be, involved in worldwide collaborations and services. For example, NBS scientists have served as presidents of the IAU Commission on Atomic and Molecular Data and as chairs of IAU working groups; NBS/NIST is the principal supplier of spectroscopy data to a worldwide network of data centers under the auspices of the International Atomic Energy Agency, Vienna; NBS writes a regular column "News on fundamental reference data" for the journal *Spectrochimica Acta B*; and the group collaborates with British, French, German, Japanese, Russian, and Swedish groups as well as several institutions in the United States on especially pressing data needs. Outside groups have often turned to NIST to find out where problems and discrepancies in the data occur and where they can assist. Parallel to the data compilation program, NIST has always maintained a cutting-edge research program in spectroscopy, since only hands-on participation with state-of the-art experimental and theoretical techniques gives NIST the authority for making thorough, realistic judgments in the critical evaluations.

Charlotte E. Moore did her Ph.D. at the University of California, Berkeley, on the spectra of sunspots, then worked at Princeton University Observatory and produced there her first comprehensive spectroscopic compilation, *A Multiplet Table of Astrophysical Interest* [5], a first edition in 1933 and a revised and greatly enlarged one in 1945. Shortly afterwards she came to NBS, where she was a member of the Atomic Spectroscopy Section until her retirement in 1968. She was married to Bancroft Sitterly, an astronomer and mathematician at American University, and was known throughout NBS as "Mrs. Sitterly." After retirement, she continued her critical compilation work at NBS into her mid-eighties and also worked for several years at the Naval Research Laboratory on the ultraviolet spectrum of the sun. During all her work, she interacted closely with spectroscopists all over the world, not only obtaining valuable additional unpublished material but also persuading the specialists to carry out more measurements and analyses that she badly needed for the tabulations. She thus exerted considerable influence on the field of spectroscopy for many years. She died in 1990 at the age of 91.

Fig. 1. Charlotte Moore-Sitterly, seated on the far right, receives the Federal Woman's Award in the White House from Lyndon B. Johnson, seated on the far left.

Charlotte Moore received numerous awards and honors, among them honorary Ph.D.s from Swarthmore College, the University of Michigan, and the University of Kiel, Germany; the Department of Commerce Gold and Silver medals; and the William F. Meggers Award of the Optical Society of America. In 1961, she was one of six women who received the first Federal Woman's Award.

W. L. Wiese received his Ph.D. in 1957 at the University of Kiel, Germany, and after working for two years at the University of Maryland, joined NBS in 1960. He started a group on plasma spectroscopy as well as the data center on atomic transition probabilities in 1962 and has led the Atomic Physics Division (formerly the Atomic and Plasma Radiation Division) since 1977. He was a Guggenheim fellow, received the A.V. Humboldt Award, the Department of Commerce Gold and Silver Medals, an honorary Ph.D. from the University of Kiel, the Distinguished Career in Science Award of the Washington Academy of Sciences, and other honors.

In recent years, William C. Martin—the leader of the Atomic Spectroscopy Group from 1962 to 1998—and his colleagues Charles Corliss, Arlene Musgrove, Joseph Reader, Jack Sugar, and Romuald Zalubas maintained the high quality of the NBS work on the atomic energy level and wavelength tables and expanded and updated much of Charlotte Moore's work. Some of their major works are cited in the selected bibliography [12-16]. W. L. Wiese and his colleagues Teresa Deters, Jeffrey Fuhr, and Georgia Martin continued the transition probability tabulations for heavier elements and also updated the tables for some light elements [17-19].

In the past few years, the NIST atomic spectroscopists combined their efforts and utilized the Internet as the new dissemination medium to establish a unified comprehensive *Atomic Spectra Database* on the World Wide

Web [20] which contains spectral reference data for 91 000 wavelengths, 45 000 transition probabilities and 70 000 energy levels, covering all natural elements (and some man-made ones up to Z=100) and—with many stages of ionization included—a total of 450 spectra. This database, with the latest version published in March 1999, has quickly become very popular, with about 45 000 hits per month and rising.

Prepared by Wolfgang L. Wiese.

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