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Atomic Physics and Spectroscopy During the First 50 Years of JPCRD

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AFFILIATIONS

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ABSTRACT

Atomic spectroscopy and atomic physics papers represent a significant part of publications in Journal of Physical and Chemical Reference Data (JPCRD). Critical compilations of spectroscopic data, accurate calculations of collisional parameters, and bibliography on spectral line profiles and shifts provided much needed information for plasma physics, astrophysics, lithography, fusion research, and other fields of science. We present a brief overview of the atomic physics research published in JPCRD over its first 50 years.

Key words: atomic physics, atomic spectroscopy, atomic collisions, spectral line shapes, data compilations.

CONTENTS

1. INTRODUCTION

In the early 20th century, atomic spectroscopy research was highly instrumental in providing the emerging field of quantum physics with the most accurate data to test new ideas and theories. At that time, even a few precise energy levels or wavelengths were often sufficient to captivate physicists' curiosity and provide the much required benchmarks. Following the explosive development of astrophysical research and plasma physics, more and more atomic data were and still are required to analyze complex spectra from neutral atoms to highly charged ions of heavy elements. This, in turn, brought about large compilations of atomic data that originally did not have many viable options for publication in "standard" scientific journals. Then, 50 years ago, the very timely appearance of the Journal of Physical and Chemical Reference Data (JPCRD) opened new pathways to report and disseminate high-quality atomic data.

As of today, there are more than 100 JPCRD papers on atomic physics covering basic spectroscopic data, collisional parameters, spectral linewidths and shifts, isotope shifts, quantum-electrodynamic effects, and so on. These papers are typically highly cited and extensively used in various fields of science where atomic data are in demand, e.g., astrophysics, high-energy-density physics, fusion research, lithography, atmospheric physics, and others. Here, we present a brief overview of the JPCRD atomic-physics papers during the first 50 years of the journal.

2. NIST evaluated data publications

Due to a strong partnership between JPCRD and the National Institute of Standards and Technology (NIST), most of the atomic papers in the journal come from the NIST Atomic Spectroscopy Group although more and more contributions from other research groups around the world are being submitted and published in recent years. Atomic spectroscopy has long been an important part of research at NIST and its predecessor, the National Bureau of Standards. One of the responsibilities of NIST is the production of physical reference data for science and industry, which is based on multi-faceted evaluations of the available scientific information. The critical evaluations of fundamental atomic spectroscopic data started with the pioneering compilations by Charlotte Moore Sitterly in the late 1940s. Her *Atomic Energy Levels* series[1–3] has become a classical example of a complete and scrupulously analyzed collection of important and vastly needed atomic data. In addition to setting various basic criteria for the data analysis, she also developed specific formats for data presentation that are still in use today. Charlotte Moore also established two data centers, on Atomic Energy Levels and on Atomic Transition Probabilities (or oscillator strengths) and Line Shapes, to carry out the compilation work and to develop and maintain databases on atomic spectroscopic data. With time it became evident that for optimal representation and utilization of data, it is preferable to rather develop unified compilations including both energy levels and radiative transition probabilities.

The primary difference between the energy level (or spectral line wavelength) and the transition probability compilations is in the availability of accurate experiments. The legacy and modern spectroscopic instruments can efficiently perform measurements of wavelengths with resolving powers exceeding 1 000 000 in the infrared or visible spectral ranges although the instrument resolution somewhat drops for extreme ultraviolet or x-ray photons. Importantly, such measurements are routine and plentiful. On the other hand, most measurements of transition probabilities are directly related to determination of spectral line intensities that are affected by experimental conditions, and therefore, they are much more demanding and less accurate—it is very challenging to measure radiative probabilities at even sub-percent level. Therefore, most of the compilations of transition probabilities are based on advanced calculations. However, this shortcoming is largely alleviated by the fact that the modern atomic theories are generally very mature. The new theoretical methods have been widely tested and benchmarked so that uncertainty quantification for various atomic systems may be carried out quite reliably.

It should also be mentioned that over the decades of critical data evaluation research, the NIST scientists developed the corresponding methods and computational tools, which are continuously improved and updated. The most recent description of the systematic approach to data evaluations can be found in Ref. 4.

The first JPCRD paper on atomic energy levels[5] was published by the Director of the Data Center on Atomic Energy Levels (Martin) in 1973. This was an update of his previous compilation on neutral helium from 1960 resulting from a number of accurately measured new spectra. The paper presented data for singly excited levels up to the principal quantum number $n = 22$, a number of doubly excited autoionizing levels, and several accurately determined ionization limits. As typical for NIST compilations, this work contains a scrupulous assessment of uncertainties for all reported atomic parameters. It is remarkable that in spite of many advances in He I spectroscopy over the last 50 years, this seminal paper is still routinely cited in the literature.

The transition probability publications in JPCRD started with an outstanding compilation of forbidden lines in the spectra of iron-group elements from V (atomic number $Z = 23$) to Ni ($Z = 28$) by Smith and Wiese.[6] The forbidden lines from highly charged ions were already well known from solar spectroscopy studies where, for instance, discovery of the famous "green" magnetic-dipole line at 530.3 nm in Fe XIV[7,8] unambiguously confirmed the extremely high temperature of about 1 000 000 K of the solar corona. In the early 1970s, a rapid advance of magnetic fusion research resulted in a high demand for new spectroscopic methods to diagnose even hotter, multi-million-degree plasmas in tokamaks and stellarators, where intensities of many forbidden lines are indeed sensitive to electron density variations. A key parameter that is crucial for determination of the appropriate range of densities is the radiative transition probability. Thus, this timely paper provided the valuable and accurate up-to-date information that is still being used in spectroscopic diagnostics of fusion devices.

Over a few decades, the atomic data compilations were strongly affected by the magnetic fusion research. For instance, the iron-group elements were important components of the early tokamak plasma-facing materials. Sputtered by energetic plasma particles, their atoms would propagate into the hot core plasmas and become ionized to very high degrees of ionization. The ensuing spectra across a very wide spectral range provided important diagnostics of plasma temperature and density. The extensive publications of energy levels and spectra (some later publications including transition probabilities) for ions of Fe,[9,10] Cr,[11,12] Mn,[13,14] V,[15,16] Ti,[17,18] Sc,[19,20] Ni,[21] and Co[22,23] as well as a very comprehensive compilation of energy levels for the iron-period elements from K to Ni[24] created a solid foundation for spectroscopy of magnetic fusion devices. This effort was complemented by a number of critical compilations of transition probabilities for Sc and Ti;[25] V, Cr, and Mn;[26] Cr;[27] Fe, Co, and Ni;[28] and Fe.[29,30] With the following measurements and calculations, those compilations were updated in 1988 for Sc through Mn[31] and Fe through Ni.[32] In addition to the iron-group elements, Mo was also of high importance for magnetic fusion since it was previously used as a first-wall material. Accordingly, a number of compilations on its spectra[33,34] were developed in the 1980s. This extensive work on fusion-related atomic spectroscopy culminated in a comprehensive compilation for Ti, V, Mn, Cr, Fe, Co, Ni, Cu, Kr, and Mo published as the JPCRD Monograph 8 by Shirai *et al.*[35]

At the present time, the magnetic fusion research aims at completion and initiation of the international ITER reactor. Its first wall will be covered by beryllium, which has just four ionization stages. The recommended energy levels and spectra for Be I[36] and transition probabilities for all ions[37] were reported in 1997 and 2010, respectively. Interestingly, the most recent JPCRD paper is devoted to the benchmark calculations of energy spectra and oscillator strengths of Be I.[38] Much more challenging is the spectroscopy of tungsten ($Z = 74$), which will be the plasma-facing material for the ITER divertor. The 2006 JPCRD paper by Kramida and Shirai[39] provided the first evaluated set of spectroscopic data for neutral and singly ionized W.

Another important consumer of atomic spectroscopic data is astronomy and astrophysics. Here, the primary interest is in relatively light elements ($Z \leq 30$) due to their high abundance in the universe. The relevant compilations of energy level data cover Al,[40,41] Ca,[42] K,[43,44] Mg,[45,46] Na,[47] Si,[48] P,[49] S,[50,51] Cu,[52,53] O II,[54] Zn,[55] Ne,[56] Ar,[57] and Na.[58] In addition, sets of critically evaluated transition probabilities for Ar;[57,59] C, N, and O[60] (followed by an improved compilation for C and N[61]); and H, He, and Li[62] were reported as well.

After the launch of the Chandra X-Ray Observatory in 1999, it became evident that the then-existing atomic data, in particular, on the radiative transition probabilities, may not provide satisfactory support for the upcoming observations. To address this problem, the NIST Atomic Spectroscopy Group generated critical compilations for S VII–XIV,[63] Si VI–XII,[64] Mg V–X,[65] and Ne V–VIII[66] supplying data for the ions emitting in the x-ray spectral range of interest to Chandra. Those compilations made use of the newest results calculated by the rapidly improving theoretical methods, including multi-configuration Hartree–Fock and Dirac–Fock theories. This work later evolved into the production of complete sets of transition probabilities for all ions of Na and Mg,[67] Al,[68] Si,[69] and S.[70]

The noble gases heavier than Ar are also often used for spectroscopic diagnostics of terrestrial and astrophysical plasmas, and therefore, the spectra of their atoms and ions have been studied in numerous publications. As a result, several data compilations for Kr[71–73] and Xe[74,75] were published in JPCRD. Another diagnostically important element, Ba, was the subject of a number of spectroscopic papers[76–78] that summarized the evolution of accurate data on energy levels and transition probabilities.

Other publications from NIST address data needs for diverse fields of physics. The 1974 paper on the ground states and ionization potentials of lanthanide and actinide atoms and ions[79] was one of the first data collections for these most complex atomic systems. Another series of papers[80–82] provided decadal updates to the binding energies of negative ions. Other publications report critically evaluated data for the elements of interest for development of atomic clocks (Rb,[83] Hg,[84] Fr,[85] Cs,[86] and Sr[87,88]), inertial confinement fusion (Ge[89] and Ga[90]), and others.[91–93]

In 2005, Sansonetti and Martin published a comprehensive compilation presenting a selection of the most important and frequently used atomic spectroscopic data in an easily accessible compact format.[94] This Handbook of Basic Spectroscopic Data includes data for the neutral and singly ionized atoms of all elements from hydrogen through einsteinium ($Z = 1$–99). The wavelengths, intensities, and spectrum assignments are given in a table for each element, and the data for ~12 000 lines of all elements are also collected into a single table, sorted by wavelength in a "finding list." Simultaneously with the JPCRD publication, the Handbook was released as an e-book as well as an online database.[95]

The development of online databases of atomic reference data was always a very important component of the atomic physics program at NIST. It was therefore very natural for the JPCRD atomic data compilations to be directly added to the NIST Atomic Spectra Database (ASD),[96] the most authoritative collection of critically evaluated atomic spectroscopic data. The ASD, which currently contains about 112 000 energy levels, 292 000 spectral lines, and 123 000 transition probabilities, is queried more than 600 000 times a year for up-to-date spectroscopic data, and its success is certainly in part due to the high quality of JPCRD contributions. Furthermore, the reference database work laid out foundations for the development of other online tools for atomic and plasma spectroscopy, e.g., Laser-Induced Breakdown Spectroscopy Database,[97] FLYCHK collisional-radiative code,[98] and NIST-LANL Lanthanide Opacity Database.[99] An extensive description of the ASD structure, evolution, and future goals can be found in the recent paper.[100]

3. Other publications on atomic physics

In addition to publications from the NIST group, JPCRD has become a journal of choice for many other research groups producing accurate atomic data, both spectroscopic and collisional. Two relatively small papers by Krause[101] and Krause and Oliver[102] on atomic radiative and radiationless yields and natural widths for K- and L-shells are among the mostly cited papers from JPCRD. For many years, Erickson's paper on one-electron atoms[103] was considered a *de facto* standard as it accurately reported up to 11 or 12 significant digits for the corresponding energy levels. A 1700-page volume by Kelly on atomic and ionic spectrum lines below 2000 Å (H through Kr)[104] was one of the most extensive compilations of x-ray, extreme ultraviolet, and vacuum ultraviolet spectra. Other papers[105–107] from the late 1970s report on infrared spectral lines,[105] electron binding energies,[106] and the B I spectrum.[107]

More recently, a number of accurate results on quantum-electrodynamic effects in muonic hydrogen,[108] bound electron g-factors in highly-charged ions,[109] helium isotope shifts[110] and accurate theoretical[111] and experimental analyses[112] of its energy structure, Lamb shifts in hydrogenic atoms,[113] fundamental data for Ra I and Ra II,[114] ionization energies of lanthanides,[115,116] and other important data[117–121] were also published in JPCRD. It is interesting to note, for instance, that the recently developed theoretical methods can surpass the experimental data for non-trivial three-electron Li-like systems.[122]

Collisional atomic data have also found their place in the JPCRD universe. In a series of three papers, Janev *et al.* reported charge-exchange cross sections for collisions of neutrals with multiply charged ions.[123–125] These data are particularly important for fusion experiments. The recommended data for ionization cross sections of light atoms and ions[126,127] published in the 1980s are still often used in advanced collisional-radiative models of plasma emission. More recent works present charge transfer cross sections in metal vapors,[128] photon- and electron-impact cross sections for atomic oxygen,[129,130] inner-shell ionization cross sections,[131] a series of papers on electron collisions with Be,[132] Mg,[133] Zn,[134] and In,[135] and recommended positron scattering cross sections.[136]

4. Line broadening and shifts

Unlike fundamental atomic parameters (energy levels, wavelengths, and transition probabilities), which are not significantly altered by plasmas in most cases, spectral line shapes and shifts are strongly affected by plasma environments. The instrumental width is due to imperfections of the recording equipment, and it can be subtracted from the measured line profiles. Then, the Doppler broadening is due to the emitter motion, and thus, it is mostly sensitive to plasma temperature. The most complicated contributions to spectral line profiles come from the plasma fields and interactions with fast and slow plasma particles. Both accurate calculations and precise measurements of such collisional widths are very elaborate, and the availability of tabulated recommended line profile parameters is always of high importance.

The JPCRD papers on line broadening and shifts were mainly due to a very fruitful collaboration between NIST and Konjević and co-workers in Belgrade, Serbia (then Yugoslavia). Already in 1976, two review works on Stark widths and shifts in non-hydrogenic atoms were released.[137,138] Those reviews were later updated several times to account for new experimental and theoretical data.[139–142] Some of the line broadening reviews contained extensive bibliographies that resulted in the development of an online bibliographic database.[143] This database currently contains more than 7000 references and it is regularly updated and expanded.

5. Conclusions

For the last 50 years, JPCRD presented researchers around the world with exceptional data in a variety of fields, including atomic physics and spectroscopy. The JPCRD atomic-physics papers are widely cited in the literature, and the reported data are critically important for diagnostics and analysis of various environments, including terrestrial and astrophysical plasmas, magnetic and inertial fusion, and lithography. In recent years, the emphasis is clearly shifting from the basic spectroscopic data (i.e., energy levels, wavelengths, and transition probabilities) to more sophisticated atomic parameters, such as isotope shifts and quantum-electrodynamic contributions. Yet, there is no doubt that JPCRD will continue to strongly influence the atomic physics research due to the uniqueness and highest quality of its publications.

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6. AUTHOR DECLARATIONS

6.1. Conflict of Interest

The author has no conflicts to disclose.

Data Availability

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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