Honoring Charlotte Moore Sitterly: Astronomical Spectroscopy in the 21st Century
Proceedings IAU Symposium No. 371, 2024
D. R. Soderblom & G. Nave, eds.
doi:10.1017/S1743921323000212

Legacy of Charlotte Moore Sitterly in the Internet Age

Alexander Kramida

National Institute of Standards and Technology, Gaithersburg, MD 20899, USA
email: `alexander.kramida@nist.gov`

Abstract. Most (yet not all) results of atomic physics research of Charlotte Moore Sitterly (CMS), which was closely connected to astrophysics, are now incorporated in online databases, one of which is the Atomic Spectra Database of the National Institute of Standards and Technology. The use of this database extends far beyond astrophysics, but this review focuses on astrophysical applications. The impact of CMS's work on modern atomic physics and other sciences is discussed, and problems that urgently need solutions are outlined.

Keywords. atomic data; standards; methods: data analysis; techniques: spectroscopic; line: identification

---

1. Introduction

This article is a somewhat extended transcription of the plenary talk I gave at the General Assembly of the International Astronomical Union on August 9, 2022, in Busan, Republic of Korea.

There are a number of excellent biographical materials describing the life and scientific career of Charlotte Moore Sitterly (CMS); see, e.g., Rubin (2010) and Martin (1991). Thus, it suffices here to give her brief Curriculum Vitae in Table 1.

I only want to make a few comments on this CV. First, the official name of CMS's first job at the Princeton University Observatory was "Computer." Carl Kessler called it "computer aide" in his article Kessler (1988). However, later on it evolved into something much more elaborate, which nowadays should be called "Data Analyst." I consider myself to hold that profession as well, and that is why I am here discussing the gigantic legacy of CMS and its evolution in the Internet age.

Second, in both her first and second jobs at the Princeton University Observatory, Charlotte's supervisor was Dr. Henry Norris Russell, a famous atomic physicist and astronomer. He made a huge influence on CMS throughout her life and career; this will be further discussed later on.

And third, not many people realize nowadays that women in science were treated unequally with men in the USA until the second half of the 20th century. Vera Rubin mentions that "Princeton's graduate school would open to special women only in 1961." Thus, despite having a brilliant scientific advisor, H.N. Russell, right there at Princeton, Charlotte had to go to University of California at Berkeley to earn her Ph.D.

Henry Norris Russell was a man of many interests, but he is most known for his contributions to atomic physics. His name is presently most often mentioned in connection with the Russell-Saunders coupling scheme, more often called *LS* coupling scheme (Russell & Saunders (1925)). The above article introduced this coupling scheme and the related atomic-physics notation. Before that article, designations of atomic energy levels and transitions between them were in total disarray in the literature. As

Table 1. Curriculum vitae of Charlotte Moore Sitterly.

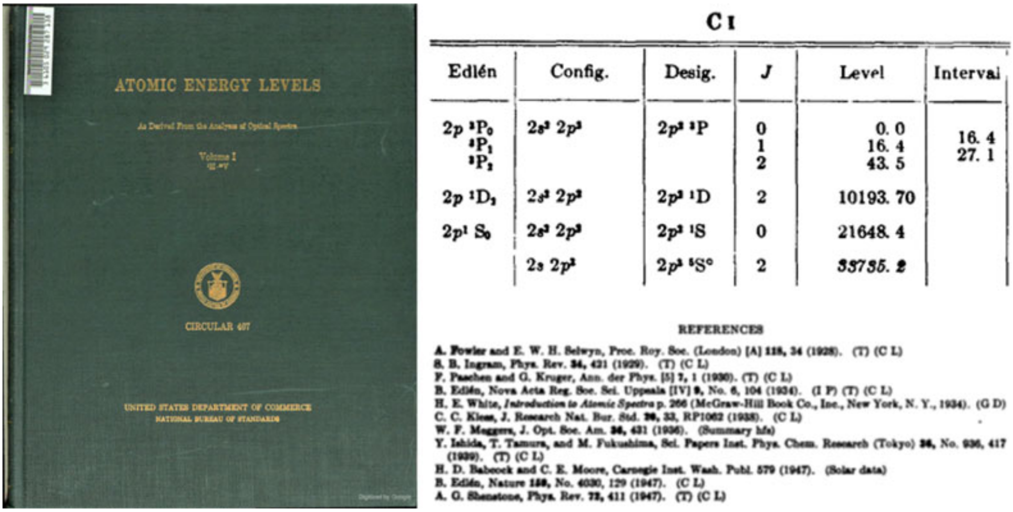
Life		1898–1990
B.A. in math	Swarthmore College, PA	1920
"Computer"	Princeton Univ. Observatory (under **H. N. Russell)**	1920–1925
"Computer"	Mount Wilson Observatory, near Pasadena, CA	1925–1931
First published paper	Moore & Russell (1926)	1926
Ph.D. in astronomy	Univ. California, Berkeley, "Atomic lines in the Sun-spot spectrum"	1931
Research Assistant	Princeton Univ. Observatory	1931–1945
Physicist	National Bureau of Standards, Washington, DC	1945–1968
Officially retired		1968
Guest Scientist	Office of Standard Reference Data, NBS, Washington, DC	1968–1971
Guest Scientist	Naval Research Laboratory, Washington, DC	1971–1978
67 publications		1926–1993

Russell & Saunders (1925) noted, "The present state of notation for spectroscopic terms is chaotic". Some authors used combinations of upper- and lower-case Latin letters and Arabic numbers, others used Greek or German letters. One of the most popular systems of notation was that of Paschen (1919) adopted for spectra of rare-gas atoms. Those various systems were largely phenomenological, reflecting empirical regularities along series of spectral lines. Conversely, the notation introduced by Russell and Saunders is based on quantum mechanics and is directly related to the physical nature of atomic energy states. This notation was developed by a group of prominent atomic physicists, which included A. Fowler, W.F. Meggers, P.D. Foote, C.C. Kiess, J.A. Carroll, H.N. Russell, and F.A. Saunders. Among this group, the most important person for CMS (besides H.N. Russell) is William Frederick Meggers, who was leading the Spectroscopy Section of the National Bureau of Standards (NBS) at that time (more about that further on).

After receiving the Ph.D. in astronomy from the University of California, Charlotte Moore returned to the Princeton astronomy department as research assistant and research associate (Kessler (1988)). A culmination of her work there was the famous multiplet table of astrophysical interest (Moore (1945)). Naturally, in this work she followed the notation of spectroscopic terms developed by Russell and others, as described above.

At the time Moore's multiplet table was published, William F. Meggers initiated a program at NBS to construct a critically evaluated data set of atomic energy levels for all experimentally studied spectra. As Kessler noted, the popular tables of atomic energy levels existing at the time (Bacher & Goudsmit (1932)) were hopelessly out of date and needed a thorough revision. A person possessing the knowledge and skills in atomic spectroscopy was needed for this job, and Russell and Shenstone at Princeton recommended Charlotte Moore as most qualified for it. The project was supported by Edward Condon, a former Princeton associate, who was director of NBS at the time. In 1945, Charlotte Moore was hired by NBS and started her monumental work on atomic energy levels (AEL). The first of the three volumes of her critical AEL compilations was published by NBS in 1949, the second in 1952, and the third in 1958. All three volumes were quickly sold out, but the demand continued, so they were reprinted by the US Government Printing Office in 1971 (Moore (1971a), Moore (1971b), Moore (1971c)). The cover page and an excerpt from the first volume are shown in Fig. 1.

From this example one can see that the level designations in AEL have a well-defined physical meaning, with the principal and orbital quantum numbers of electronic subshells,



C I

Edlén	Config.	Desig.	*J*	Level	Interval
$2p\ ^3P_0$ $^3P_1$ $^3P_2$	$2s^2\ 2p^2$	$2p^2\ ^3P$	0 1 2	0.0 16.4 43.5	16.4 27.1
$2p\ ^1D_2$	$2s^2\ 2p^2$	$2p^2\ ^1D$	2	10193.70	
$2p^1\ S_0$	$2s^2\ 2p^2$	$2p^2\ ^1S$	0	21648.4	
	$2s\ 2p^3$	$2p^3\ ^5S^\circ$	2	*33735.2*	

REFERENCES

A. Fowler and E. W. H. Selwyn, Proc. Roy. Soc. (London) [A] **118,** 34 (1928). (T) (C L)
S. B. Ingram, Phys. Rev. **34,** 421 (1929). (T) (C L)
F. Paschen and G. Kruger, Ann. der Phys. [5] **7,** 1 (1930). (T) (C L)
B. Edlén, Nova Acta Reg. Soc. Sci. Upsala [IV] **9,** No. 6, 104 (1934). (I P) (T) (C L)
H. E. White, *Introduction to Atomic Spectra* p. 266 (McGraw-Hill Book Co., Inc., New York, N. Y., 1934). (G D)
C. C. Kiess, J. Research Nat. Bur. Std. **20,** 33, RP1062 (1938). (C L)
W. F. Meggers, J. Opt. Soc. Am. **26,** 431 (1936). (Summary hfs)
Y. Ishida, T. Tamura, and M. Fukushima, Sci. Papers Inst. Phys. Chem. Research (Tokyo) **36,** No. 936, 417 (1939). (T) (C L)
H. D. Babcock and C. E. Moore, Carnegie Inst. Wash. Publ. 579 (1947). (Solar data)
B. Edlén, Nature **159,** No. 4030, 129 (1947). (C L)
A. G. Shenstone, Phys. Rev. **72,** 411 (1947). (T) (C L)

Figure 1. The cover page and and an excerpt from the first volume of C.E. Moore's Atomic Energy Levels (Moore (1971a)).

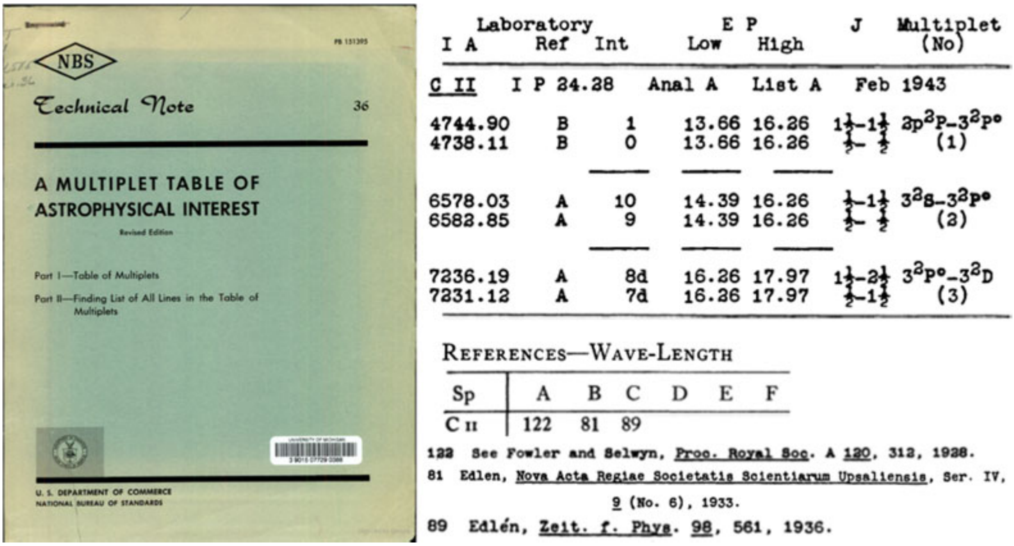
as well as the multiplicity, S (two times spin plus one), orbital momentum (L), and total angular momentum (J) quantum numbers of the final term ^SL_J. The energies are counted from the ground level, which has a zero energy by definition in this system. This is the standard established by Moore's AEL. Before that, many authors counted the atomic energies from the first ionization limit, which was intrinsically imprecise, since the ionization energy cannot be measured as accurately as the excitation energies from the ground level. In AEL, the table of levels for each spectrum is accompanied by a review of the critical evaluation and a list of references on which the evaluation of energies was based. Many of the spectra in AEL were analyzed by CMS from unpublished sets of measured wavelengths privately communicated to CMS by researchers.

Recognizing the importance of the Multiplet Table (MT) for astrophysics and other applied sciences, NBS has reprinted it in 1959 as NBS Technical Note 36 (see Fig. 2)) and later in 1972 as volume 40 of the National Standard Reference Data Series (Moore (1972b)).

In Fig. 2 one can see the layout of the tables with which most astrophysicists and atomic physicists are very familiar: each observed wavelength is accompanied by a reference to its source, an observed intensity, lower and upper energy levels (called "excitation potentials" and given in units of eV in MT), total J values of the levels, and designations of the lower and upper configurations of the multiplet. This information can be matched with the energy level data in the AEL tables.

Throughout her career at NBS, in parallel with her work on AEL compilations, CMS had continued to compile, update, and extend her atomic multiplet tables Moore (1965), Moore (1967), Moore (1968a), Moore (1968b), Moore (1970), Moore (1971d), Moore (1972a), Moore (1972b), Moore (1975), Moore (1976), Moore (1979), Moore (1980), Moore (1982), Moore (1985). The last revision of her data collections for hydrogen, carbon, nitrogen, and oxygen atoms and ions was published after her death with extensive help of Jean W. Gallagher (Moore (1993)). All these publications, including the original Multiplet Table of Astrophysical Interest (Moore (1945)), are collectively called "MT" in the subsequent text.

One paper of Russell & Saunders (1925) could not change the many ways used by atomic spectroscopists around the world. It is largely due to the popularity of the MT



PB 151395

NBS

Technical Note 36

A MULTIPLET TABLE OF
ASTROPHYSICAL INTEREST

Revised Edition

Part I—Table of Multiplets

Part II—Finding List of All Lines in the Table of Multiplets

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

Laboratory I A	Ref	Int	E P Low	 High	J	Multiplet (No)
C II	I P 24.28		Anal A	List A	Feb 1943	
4744.90	B	1	13.66	16.26	1½–1½	3p^{2}P–3^{2}P°
4738.11	B	0	13.66	16.26	½–½	(1)
6578.03	A	10	14.39	16.26	½–1½	3^{2}S–3^{2}P°
6582.85	A	9	14.39	16.26	½–½	(2)
7236.19	A	8d	16.26	17.97	1½–2½	3^{2}P°–3^{2}D
7231.12	A	7d	16.26	17.97	½–1½	(3)

REFERENCES—WAVE-LENGTH

Sp	A	B	C	D	E	F
C II	122	81	89			

122 See Fowler and Selwyn, Proc. Royal Soc. A 120, 312, 1928.

81 Edlen, Nova Acta Regiae Societatis Scientiarum Upsaliensis, Ser. IV, 9 (No. 6), 1933.

89 Edlén, Zeit. f. Phys. 98, 561, 1936.

Figure 2. The cover page and and an excerpt from the first reprint of C.E. Moore's Multiplet Table of Astrophysical Interest (Moore (1945)).

and AEL publications of CMS that atomic physicists now speak the same language and can understand one another, with the same system of notation used by everyone.

This system of atomic spectroscopy designations and terminology was further developed and standardized by physicists at NBS, most notably by William Clyde Martin Jr., who succeeded W.F. Meggers as the Chief of Atomic Spectroscopy Section of NBS in 1968 and served at this position until 1998. In 1988, NBS was reorganized and renamed as National Institute of Standards and Technology (NIST). W.C. Martin's position was renamed as Leader of Atomic Spectroscopy Group (ASG). Martin has recognized importance of another atomic parameter, transition probability (or a related quantity, oscillator strength) for applications in astronomy and other sciences where plasma diagnostic plays a major role. Elemental abundances in stars are derived from oscillator strengths of observed atomic transitions. Thus, the activities of ASG were extended by measurements and critical compilations of atomic transition probabilities. This line of research was headed by Wolfgang L. Wiese. Together with Wiese, Martin has published his now classical review article about basic ideas, notation, data, and formulas in atomic spectroscopy (Martin & Wiese (1996)), which is nowadays the ultimate reference for atomic-spectroscopy notation and terminology.

2. Critical compilations

Charlotte Moore was a pioneer in developing the procedure for critical compilation of atomic data. This procedure has been refined later by the members of the ASG at NIST. A modern version of the workflow of a critical compilation procedure is shown in Fig. 3. Several versions of this diagram were developed at NIST and presented by members of the ASG at various conferences (Reader (2006), Kramida (2007), Kramida (2011), Kramida (2013)). Compared to these previous versions, the present scheme is extended by inclusion of calculation and compilation of transition probabilities, as well as reduction of all observed intensities to a common scale. These procedures are integral in evaluation of correctness of spectral line identifications.

The diagram depicted in Fig. 3 shows two sets of input observational data. Typically, there are many more publications with experimental data on each spectrum. At the time

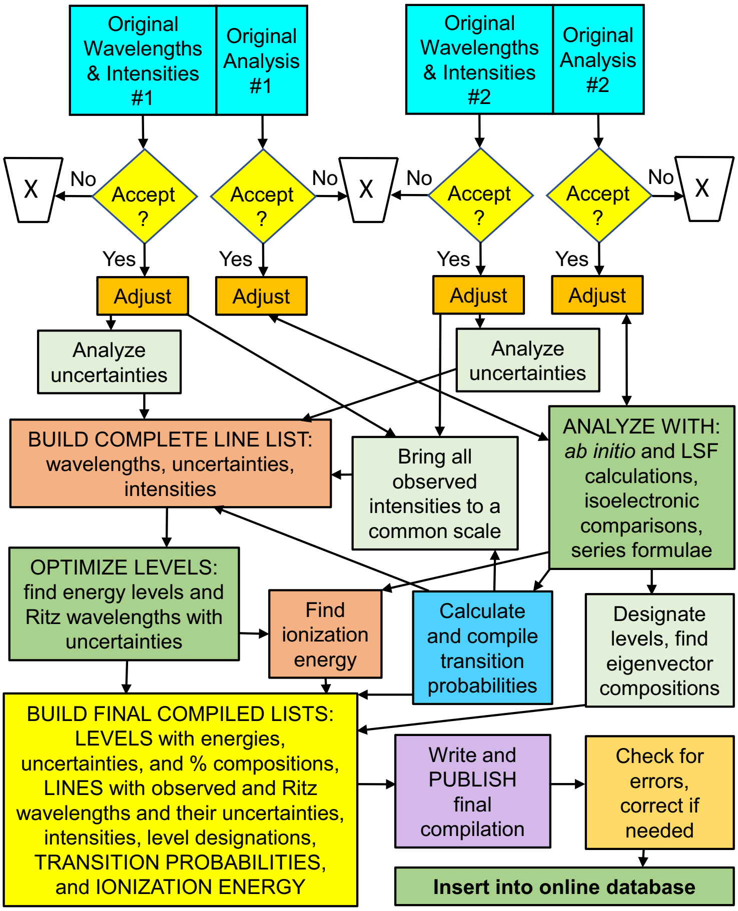


Figure 3. The workflow of a critical compilation of an atomic spectrum data, as currently used by the Atomic Spectroscopy Group at NIST.

CMS made the first critical compilations, there were on average about three experimental studies per spectrum. Nowadays, the average number is 17 papers per spectrum (see more on this topic further below). For many spectra, these studies were unpublished at the time CMS was working on AEL compilations; their results were privately sent to her by researchers from around the world. The different studies are usually fragmentary: they cover limited ranges of spectrum or ranges of energies of excited states. The most difficult part of the critical compilation process is reconciliation of contradicting parts of these fragmentary studies. That is where the theoretical calculations, isoelectronic comparisons, fits with series formulas, and other methods of analysis are indispensable. The main goal of this analysis is to construct a global list of the best measured wavelengths with energy-level classifications and relative intensities for each observed line. From this line list, a set of optimized level values is derived, which best fits all observed wavelengths. These level and line lists are published as recommended data sets. At the time of CMS's work on AEL, this was the final step of the process. Nowadays, after an additional error-checking step ensuring the internal consistency, these data sets are inserted in an online database. For this purpose, the NIST ASG uses the Atomic Spectra Database (ASD; Kramida *et al.* (2021)).

Some of the blocks depicted in Fig. 3 involve very complicated work. For example, a critical compilation of transition probabilities for a spectrum is in itself a complex process first described by (Wiese (1996)) and further developed by the present author (Kramida (2013)). Thus, a critical compilation of a complete set of spectral data for an atomic spectrum is a very time-consuming procedure. At the time when CMS did her work on AEL, when only a few data sources were available, and transition probabilities were left out of the picture, it took her about 10 days per spectrum on average. Nowadays, with much more data published, with much increased measurement precision, and increased complexity of the spectra, it typically takes more than a year to compile a single spectrum. For example, the recently published critical compilations of the C I and C II spectra (Haris & Kramida (2017); Kramida & Haris (2022)) took about five years each to complete.

A critical compilation becomes obsolete almost immediately after it is published, since new experimental data on atomic spectra continue to be published at a rapid pace (more on that further below). Even if a single wavelength is remeasured with increased precision, the new measurement cannot simply replace the previous one in a critically evaluated data set. This is because each wavelength is part of a self-consistent picture involving all measured transitions and energy levels. Changing one wavelength requires the entire data-reconciliation process to be repeated, which is impossible to do as soon as the new data are published.

3. Bibliographic databases

The starting point of each compilation is collection of bibliographic records and copies of original papers. In 1968 and 1969, CMS had published the bibliography she used in her work (Moore (1968c), Moore (1969a), Moore (1969b), Moore (1969c)). This bibliography includes 605 references. CMS had developed a system of indexing the papers using special search keywords, such as “CL” for classified lines, “WL” for wavelengths, “IP” for ionization potential (nowadays, more properly called ionization energy), “IS” for isotope shift, “hfs” for hyperfine structure, “ZE” for Zeeman effect, and “Osc.Str” for oscillator strengths. This system of keywords, in a somewhat revised and extended form, was later adopted as the basis for indexing the bibliography on atomic spectra that continued to be collected by the ASG at NBS and further at NIST (Hagan & Martin (1972), Hagan (1977), Zalubas & Albright (1980), Musgrove & Zalubas (1985)). However, it was decided that bibliography on oscillator strengths (and transition probabilities) should be collected separately from literature on atomic structure and wavelengths. This task was first taken on by W.L. Wiese, who started working at NBS in 1960 and continued to head the transition probability data section of the ASG at NIST until his retirement in 2004. The first collections of bibliography on transition probabilities were published under his supervision from 1962 to 1973 (Glennon & Wiese (1962), Glennon & Wiese (1966), Glennon & Wiese (1968), Miles & Wiese (1970), Fuhr & Wiese (1971), Fuhr & Wiese (1973)). This bibliographic work was continued by another member of this section, Jeffrey R. Fuhr (Fuhr *et al.* (1978a); Miller *et al.* (1980)). In parallel, Wiese and Fuhr were collecting and publishing a bibliography on atomic line shapes and shifts (Fuhr *et al.* (1972), Fuhr *et al.* (1974), Fuhr *et al.* (1975), Fuhr *et al.* (1978b), Fuhr & Lesage (1993)).

After 1993, these bibliographies continued to be collected, but NIST stopped publishing them on paper. It was only in 2010 when all collected references were transferred into a newly created bibliographic data system containing the three online bibliographic databases, separately for atomic energy levels and spectra (Kramida (2010a)), atomic transition probabilities (Kramida & Fuhr (2010b)), and line broadening and shifts (Kramida & Fuhr (2010c)). Although the references to these three databases all have

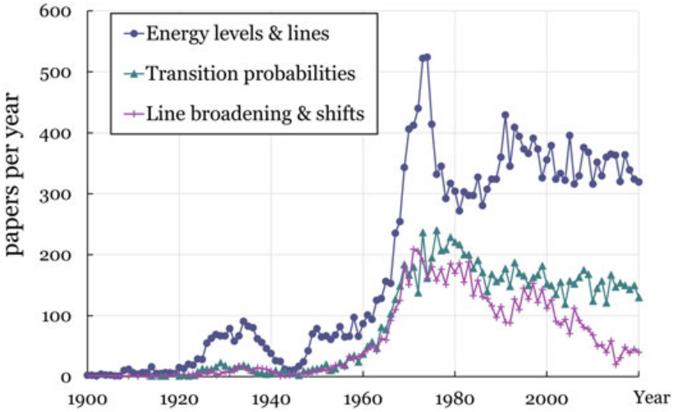


Figure 4. Number of papers with atomic spectroscopy data published per year, assessed by counts of records in the three NIST bibliographic databases (Kramida (2010a); Kramida & Fuhr (2010b,c)).

a fixed year 2010, they are actually updated weekly and thus provide complete and concurrent lists of publications for each spectrum. The elaborate systems of search keywords developed by CMS, W.L. Wiese, and J.R. Fuhr had been adapted to accommodate online user requests and implemented in a relational database management system. A complicated but semi-automatic procedure had been developed by the present author to retrieve new relevant publications from the Internet. These three online databases now constitute a robust basis for all ongoing critical compilations of atomic spectra at NIST.

Completeness of the lists of publications is ensured by checking the lists of references in newly published papers. In parallel with NIST, the Institute for Spectroscopy of the Russian Academy of Sciences in Troitsk, Russia, also maintains an online bibliographic database on atomic spectra called BIBL (Kramida *et al.* (1987)), which is updated once or twice a year. Checking this database once a year is an additional means of ensuring completeness of the NIST bibliographic databases. A 100 % completeness can never be guaranteed. Some papers inevitably are missed, especially when the valuable spectroscopic data are not mentioned in the abstract or presented in tables, or when they are hidden in supplemental materials, or when the publication source is not indexed in the Web of Science database (Clarivate (2022)), which is the main source of the NIST bibliographic information. Nevertheless, the lists of publications retrieved from the NIST bibliographic databases provide a very good starting point for any spectrum analysis.

4. The scope of work

It is interesting to compare the scope of work that CMS was facing in her AEL and MT compilations with that tackled by the NIST ASD team.

At present, there are about 35,000 papers on atomic spectroscopy stored in the NIST bibliographic system. More than 95 % of these papers contain numerical spectral data. This should be compared with the total number of references in CMS's bibliographic records (Moore (1968c), Moore (1969a), Moore (1969b), Moore (1969c)), which is about 2500. For the last 20 years, new papers with atomic spectroscopy data continue to be published at a steady pace of about 400 papers per year. This is illustrated in Fig. 4.

It is clearly seen from Fig. 4 that the volume of published data available to CMS (prior to 1960) was much smaller than now. To create the three AEL volumes, she labored for 13 years, making her publication-processing rate to be about 200 papers per year. Assuming the same (very high!) productivity and the same time period of 13 years, to

Table 2. Numbers of studied atomic spectra and numbers of publications on them at the time of Charlotte Moore Sitterly's work compared with the present time.

	All spectra	**Spectra with level & line data**		
		All ions	Atoms	1^{st} ions
Moore's bibliography (1969), ≈2500 papers				
Number of spectra:	605	465		
Average papers per spectrum:	5	≈3		
Range:	1–54	1–40		
NIST Bibliographic Databases (2022), ≈35,000 papers				
Number of spectra:	**7151**	**2665**		
Average papers per spectrum:	**23**	**17**	**95**	**51**
Range:	1–1399	1–389	3–389	1–183

update her compilations by critically reviewing the 35,000 papers available today (plus the projected 5000 new papers that will be published within this time period), it would take 15 equally productive workers. With a group size smaller than three persons, the work is impossible to complete, as there are more newly published papers each year than such a group could review. This is the present situation with ASG.

One can see in Fig. 4 that the only atomic spectroscopy area exhibiting a significant decline of activity is line broadening and shifts. These parameters are less important for spectrum analysis than wavelengths and transition probabilities. However, they are important for modeling of astrophysical spectra, especially considering the greatly increased spectral resolution of the modern astrophysical instrumentation, so the decline of this area of research is of great concern for astronomers.

Table 2 compares the numbers of studied atomic spectra and publications on them at the time CMS did her research with those at present time. CMS's bibliography included, for each spectrum, not only references for energy levels, measured wavelengths, line classifications, and ionization energies, but also references to studies of hyperfine structure, isotope shifts, and transition probabilities. It includes references to studies of 605 atomic spectra. Out of this total number, only 465 atomic spectra had numerical data on energy levels and spectral lines.

In CMS's bibliography, the number of references (of all kinds) per spectrum ranges between 1 and 54 with an average of about 5.

The present-day statistics represented by counts of records in one of the NIST bibliographic databases (Kramida (2010a)) are shown in the bottom part of Table 2 (although the total count of unique references, ≈35,000, is for all three NIST databases). The total number of spectra for which some published papers contain data (for any atomic parameter) is 7151, but only for 2665 of them the publications include observed energy levels and/or spectral lines. Out of these, only 1150 spectra are present in the NIST ASD (Kramida *et al.* (2021)), i.e., have either level or line data sets in this database (this number excludes the spectra for which only the ground level and/or ionization limit are given in ASD). The number of spectra for which there are some lines with energy-level classifications is even smaller, only 873. Of these, 697 spectra have some transition probabilities included in ASD. Many of these data sets are badly outdated and need to be revised. Thus, one can see that there is a tremendous amount of work needed just to assess the already published information on more than 1500 spectra. The average number of papers containing observed lines and energy levels published for each spectrum is now 17, about six times greater than at the time of the AEL work of CMS. These numbers vary between 1 and 389. They are the largest for the neutral and singly ionized atoms, for which the average numbers of papers per spectrum are 95 and 51, respectively.

This comparison again indicates that the volume of work faced by the NIST ASD team is at least several times greater than what CMS was dealing with. In fact, it is even greater because of the increased complexity of the analyses stemming from increased precision of measurements, increased numbers of observed spectral lines, involvement of transition probability analyses, and the general increase in complexity of atomic structures studied nowadays. With the present-day number of workers and the present rate of new publications on atomic spectra, it is impossible for this team to provide critically evaluated data on all spectra of interest within a reasonable time frame. In the preface to the first edition of MT, CMS wrote, “The preparation of a Multiplet Table that will meet the needs of astrophysicists both now and in the future is an almost overwhelming undertaking” (Moore (1945)). Nowadays, such an undertaking appears to be impossible to succeed if carried out by any small group of experts. This calls for a change in paradigm of the atomic spectroscopy research community: the researchers must take upon themselves the task of critical evaluation of not only their own research, but also the published research of all other authors on the same spectrum. The methodology of these critical evaluations has been developed at NIST and described in fair detail, e.g. in Kramida (2013). Fragmentary studies will inevitably be published, as such publications are often necessary for academic research. However, whenever possible, they should be planned as a part of a larger project culminating in a complete revised data set for the studied spectrum.

From the point of view of astrophysics, the situation with critically evaluated data is not that bad. If one restricts the scope of atomic spectra to those 603 that are of most interest for astrophysicists, i.e., those with nuclear charge $Z \leqslant 30$ and those with $Z \leqslant 99$ and ion charge $q \leqslant 2$, one finds that NIST ASD contains some data for 594 of these spectra. Only one of the missing spectra, Np II, has some published data on classified lines and energy levels. For 514 astrophysically important spectra, ASD has sets of spectral lines with energy-level classifications, and 486 of them have data on transition rates. Thus, in regards to serving the astrophysical community, the focus of the ASD team should be (and in fact, is) not on inclusion of more ions but on improvement of already existing data sets. In the past ten years, the NIST ASD has greatly extended and improved its content for spectra of neutral and moderately charged atoms with $Z \leqslant 30$, with the number of classified lines and critically evaluated transition probabilities increased by several tens of thousands.

5. Uses and users of atomic spectral data

The data collected by CMS in her AEL compilations have nowadays been completely assimilated in several online databases. This assimilation began in 1993, when Daniel E. Kelleher of the NIST ASG started creating the first electronic version of an atomic spectra database system. He created a specialized database management system (DBMS) written in the C language. The first version of ASD was distributed on diskettes and included that DBMS. In parallel, the first online version of ASD was developed and released in 1995 (Martin *et al.* (1995); see also Dalton *et al.* (1998)). The lists of spectral lines originally compiled by CMS in the MT publications have never been fully included in ASD or any other online database. Instead, the first versions of ASD included a limited selection of the strongest lines of 99 elements (Reader *et al.* (1980)), complete line lists for a few spectra from NIST compilations superseding the MT data, and for a few spectra, data from Kelly’s book (Kelly (1987)), which were not critically evaluated by NIST.

Version 3 of ASD was released in 2005 (Ralchenko *et al.* (2005)). In this version, the database management system had been completely replaced, and a new interface had been developed. New graphical capabilities had been added as well. A complete account of development of the NIST ASD can be viewed in the Version History of this database accessible from its front page (Kramida *et al.* (2021)). In total, 39 versions of ASD had been released in the period from 1995 to 2021.

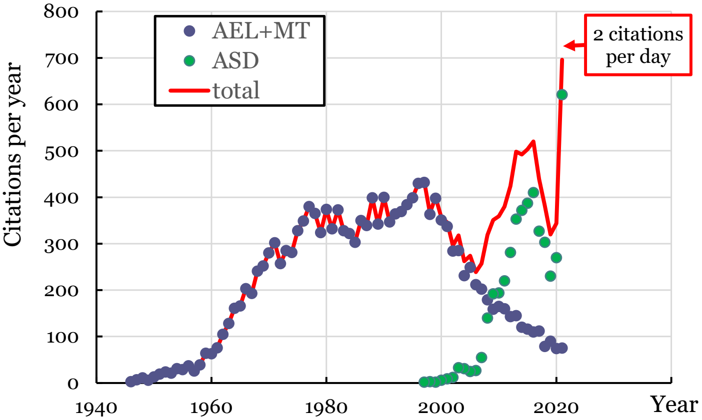


Figure 5. Number of citations to CMS's AEL and MT publications (Moore (1971a), Moore (1971b), Moore (1971c), Moore (1945), Moore (1965), Moore (1967), Moore (1968a), Moore (1968b), Moore (1970), Moore (1971d), Moore (1972a), Moore (1972b), Moore (1975), Moore (1976), Moore (1979), Moore (1980), Moore (1982), Moore (1985), Moore (1993)) and to the NIST ASD (Kramida *et al.* (2021)) per year, from the Web of Science database (Clarivate (2022)).

In parallel with the development of ASD, several other online atomic and molecular databases began to emerge. Nowadays, there are more than a dozen of them, and new ones continue to to pop up. Many of these databases have been built up starting with some version of the NIST ASD, extending it according to their specialized needs. Thus, CMS's data already assimilated in the NIST ASD continue to propagate to these new databases. It becomes virtually impossible now to trace the use and impact of CMS's data products through these multiple Internet resources. In the subsections below, an attempt is made to trace CMS's impact through direct citations to her AEL and MT works in the literature, as well as citations to the NIST ASD and an analysis of statistics of user requests to this one database.

5.1. *Citations in literature*

Fig. 4 shows the trends of citation rates for CMS's AEL & MT publications and for NIST ASD. It should be noted that complete and accurate counts of citations are virtually impossible to obtain for these sources. For example, citations to the three AEL volumes (Moore (1971a), Moore (1971b), Moore (1971c)) are spelled in the literature in about 2500 different ways, while the Web of Science database (Clarivate (2022)) allows tracking citations for not more than 2000 papers.

Citations of NIST ASD have similarly too many different forms, sometimes hard to recognize. Nevertheless, I am confident that that the citation data presented here and further below are reasonably accurate.

One can clearly see from Fig. 5 that after the advent of NIST ASD in 1995 researchers gradually switched from quoting CMS to NIST ASD (quite often, other online databases are quoted, but this is not reflected in the plot). As explained above, much of the energy level data taken from NIST ASD are actually CMS's data from AEL, but citations cannot reflect it in any way, unless the researchers are careful and accurate in quoting the data they take from ASD. This database provides references to the original source of the data, as well as the "primary source," which may be a compilation such as AEL. Unfortunately, not many researchers are careful enough in quoting other research.

Thus, a large part of citations of the online databases actually pertain to CMS's legacy, mainly AEL. The continuous line in Fig. 5 is a sum of citation numbers for NIST ASD and those for AEL & MT, and it roughly represents the total trend of use of CMS's data in the literature. As one can see, the citation rate is growing, now approaching two citations per day.

According to the Web of Science data (Clarivate (2022)), the AEL volumes of CMS have attained about 15,000 citations in 78 fields of science. Only 2.4 % of these citations are from astrophysics. The number of citations of her MT publications is three times smaller, but more than half of them are from astrophysics. An interested reader can find more details on this subject in the Appendix.

5.2. *Online user queries statistics*

Not all research results in publications in open literature. Thus, counts of citations necessarily miss some research that uses the data of CMS and other reference data sources. In the Internet age, a potentially better way to assess the use of data is to analyze the statistics of online user requests to databases. However, it is much more difficult for an open-access database such as NIST ASD, where the users can only be identified by their internet addresses. To figure out what field of research and what institution the user belongs to, one can make a reverse domain name server lookup and associate the domain names with institutions. This task is difficult to automate, and many internet addresses do not tell anything useful, as they belong to general Internet service providers rather than to scientific institutions.

In 2011–2012, the NIST ASD team made a research of user queries to the ASD database. Its main results were presented in an online news article (Suplee & Kramida (2012)). Although nearly half of all user requests for ASD data came from academic institutions, and for 41 % of requests it was not possible to directly track their origin, there were sufficiently large numbers of requests that could firmly be attributed to industry, government and military institutions, and astrophysical departments and observatories. These different categories of users had distinctly different profiles of their search queries in terms of chemical elements requested. These distinct profiles allowed an indirect determination of the origin of requests coming through internet service providers or hosting companies.

The top left panel of Fig. 6 shows the proportions of users of NIST ASD Kramida *et al.* (2021) among five categories: academic institutions (universities and colleges plus international agencies and foreign institutions for fundamental research), industry, government agencies, astrophysical community, and military institutions. According to this statistic, astronomers constitute only 6 % of all users of ASD. The broad category of 'industry' includes a large number of different fields of applied research, as shown in the top right panel of Fig. 6. An interesting finding of this research was that the profile of user requests per chemical element for academic users is virtually identical to that of the users from industry. This strongly suggests that academic users, which constitute three quarters of all ASD users, are working mainly on the same topics as those that are of interest to applied research. Thus, it is fair to assume that the proportions of industrial users shown in the right top panel of Fig. 6 roughly represent the interests of the majority of ASD users, including the academic ones. Then one can say that the energy industry (including petroleum industry and fusion energy research) represents about 13 % of all users of ASD, while smaller shares of users belong to the instrumentation industry (12 %), health industry (10 %), materials research (9 %), semiconductor industry (8 %), mainly aimed at production of smaller and better chips for more powerful computers, aerospace engineering (7 %), applied research in defense (7 %), electronic

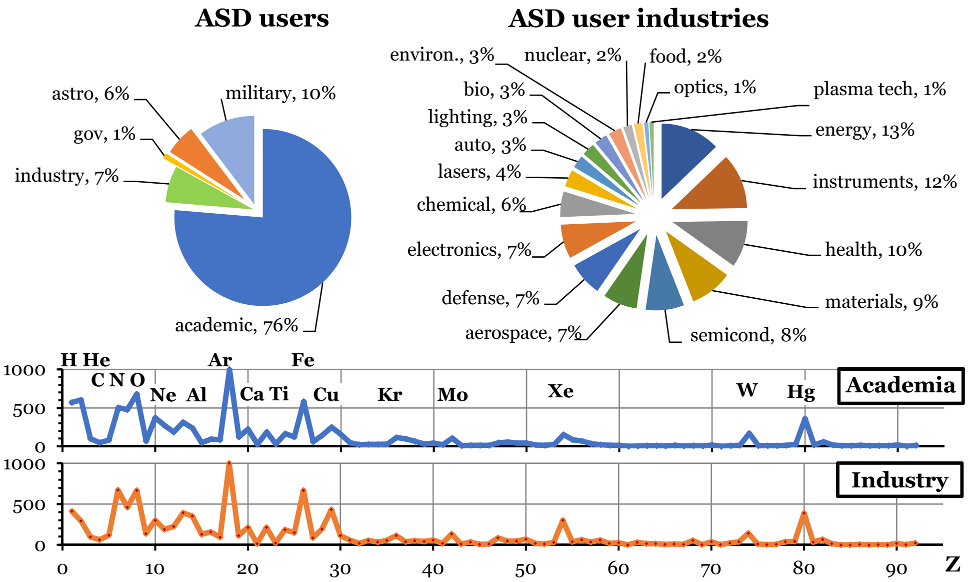


Figure 6. Top left: Shares of five categories of users in total counts of user requests to NIST ASD. Top right: Shares of different industries among the 7 % of ASD users that belong to the 'industry' category. Bottom: Shares of user requests to ASD per chemical element for users from academic institutions (upper plot) and from industry (lower plot). See text for explanation how these plots were made.

(7 %), and chemical (6 %) industries, and even smaller shares of users come from applied research in laser, automotive, lighting, and biomedical industries, environmental protection, nuclear engineering, food production, optics, and plasma technology (including welding).

6. The role of atomic spectroscopy data in the Universe

Although the previous section showed that astronomers constitute only a few percent of all users of fundamental atomic spectroscopy data, they are the most important users for NIST ASD. This is because their data needs are unparalleled in terms of their diversity and precision. Spectra of astrophysical objects contain emission and absorption features of practically all elements of the Periodic Table. In some astrophysical environments (e.g., solar corona), temperatures are so high that the atoms can be stripped of most of their electrons, so the observed emission spectra include lines from almost all ionization stages of the atoms. With the advent of cross-dispersion echelle spectrographs flown on space missions, the measurement precision now surpasses the accuracy of much if not most of currently available laboratory data. At the same time, the tasks facing the modern astrophysical spectroscopy are incredibly important: deducing the evolution of the Universe and the origin of chemical elements in the stars, answering the questions of possible variability of fundamental constants in space and time, and finding habitable exoplanets. All these tasks are very data-intensive and require high-precision reference data for atomic spectra.

Nowadays, when young students ask me why they should study atomic spectroscopy and work in this field, I semi-jokingly answer that atomic spectroscopists are responsible for the fate of the Universe. This answer has two possible meanings. One, we are responsible for the currently popular (and possibly incorrect) view on the construction and dynamics of the cosmos (from the Big Bang to formation of stars and galaxies and

https://doi.org/10.1017/S1743921323000212

future projections of their fate) and two, assuming that this current interpretation is valid, we must literally save the Universe from its imminent death by inventing some presently impossible solution.

Indeed, most of what we know about the workings of the Universe comes from observation and interpretation of spectral lines. For example, we measure the wavelengths and deduce the speed of recession of the far-away stars. These wavelengths are compared with a poor-quality reference data set, most of which comes from data measured 50 or 100 years ago, plagued by largely unknown statistical and systematic errors. That is how we currently “know” that the expansion of the Universe is accelerating. From measurements of intensities of spectral lines, astronomers deduce elemental abundances and derive the mechanisms of nucleosynthesis in stars. From these and other observations, cosmologists deduce the history of evolution of the Universe since the Big Bang and make projections into distant future. In my view, correctness of these projections is very important, and atomic spectroscopy plays a fundamental role in furnishing the data required for correct derivation of key parameters of cosmological models.

7. Some of the most important problems for astronomy and atomic spectroscopy

7.1. *Variation of fundamental constants*

One of the most data-intensive problems in modern astrophysics is to find out if the fundamental constants derived from modern terrestrial observations are really universal constants or vary in space, in time, or in super-strong gravitational fields such as those encountered near the surface of white dwarf stars. These questions are being actively investigated by several teams; see, e.g., Webb *et al.* (2011); Pinho & Martins (2016); Wilczynska *et al.* (2020); Hu *et al.* (2021). These studies are very demanding in the quality of the atomic reference data. Close attention to systematic errors is key to resolving some of their contradictions. In addition to higher-precision reference wavelengths for a broad range of atomic spectra, these studies also need careful wavelength calibration of the space-flown spectrographs (see, e.g., Hu *et al.* (2021)). Such calibration usually relies on precisely measured wavelengths emitted by a few selected atomic species, such as thorium and argon.

7.2. *Cosmic origin of heavy elements*

Another outstanding puzzle needing solution is the origin of heavy elements in the Universe. Even in the solar system, abundances of such elements as lanthanides and actinides are impossible to explain with the currently accepted models of stellar nucleosynthesis. Moreover, there are many known stars with a much more peculiar chemical composition. As Gopka *et al.* (2005) wrote in the Introduction to their article, “In 1961 Przybylski (1961) discovered a star with properties that placed it far outside of the known limits of the stellar peculiarity.” Gopka *et al.* (2005) made several conclusions in their study:

- All heavy radioactive elements with $Z = (84–99)$ except At ($Z = 85$) and Fr ($Z = 87$) are present in Przybylski’s star (PS; its astronomical label is HD 101065).
- Lanthanides are overabundant in PS by 4–5 dex compared to the solar system.
- The number of lanthanide lines with known oscillator strengths is still insufficient for accurate determination of their abundances in stars.
- Nucleosynthesis of heavy elements is an open question both in theory and in experiment.

One of the promising ideas about the possible phenomena that could produce large amounts of heavy and superheavy elements is mergers of binary systems involving neutron stars and/or black holes. Recently, electromagnetic emission across a wide range of spectrum was observed (Abbott *et al.* (2017a)) immediately following the observation of gravitational waves from a neutron star merger (Abbott *et al.* (2017b)). Such observations may provide a proof of concept that these merger events can produce large amounts of lanthanides and actinides. They spurred a number of theoretical atomic-spectroscopy studies aimed mainly at calculation of opacities of a few-times ionized elements of these two groups. This focus is due to the fact that the ejecta from NS mergers are coming out of the merger at a high fraction of the speed of light and it is not possible to spatially resolve the spectra coming towards us from those going away. So, the emitted or absorbed spectral lines are strongly broadened and merged into a quasi-continuum spectrum. Perhaps, in some geometries, observations of sharp spectral lines may be possible. This would enable detailed identifications of line spectra and determination of abundances of individual elements, provided that the wavelengths of spectral lines and their transition probabilities are known sufficiently well. So far, this knowledge is far from sufficient for both lanthanides and actinides. Volume III of CMS's AEL (Moore (1971c)) did not contain any data for lanthanides except La I–III, and any data for actinides except for Ac I–III. In the preface to this volume, A.V. Astin, who was the Director of NBS at the time, wrote that the spectra of Cerium ($Z = 58$) through Lutetium ($Z = 71$) and Thorium ($Z = 90$) through Fermium ($Z = 100$) remain for Volume IV of AEL, which is yet to be published and will be the most difficult part of the program. However, this volume never emerged. Instead, the energy levels of lanthanides were compiled by Martin *et al.* (1978), but no comprehensive line lists have been constructed for these elements.

As for the actinides, a complete critical compilation of their spectral data was never undertaken. For Ac I–III, the level designations, line classifications, and transition probabilities were recently revised (Kramida (2022)) and will be updated in the next release of NIST ASD (Kramida *et al.* (2021)) this Autumn. The Th I-III spectral data were greatly extended and revised by Redman *et al.* (2014) and inserted in the NIST ASD in 2015 (13387 lines for Th I, 6502 for Th II, and 227 for Th III). However, the transition probabilities have not been critically compiled. Thus, there are none in ASD for the thorium spectra, although some are available in the literature (see Kramida & Fuhr (2010b)). For the rest of the actinides, ASD contains limited selections of strongest lines of the first two spectra of Pa ($Z = 91$) through Es ($Z = 99$) that were included in the Reader *et al.* (1980) compilation without energy-level classifications, but no energy level tables are available in ASD for these spectra. Data on energy levels of these spectra that were available prior to 2000 had been collected in France in the Actinides database by Blaise & Wyart (2006), which also contains small selections of classified spectral lines of these spectra. A few spectral lines and energy levels of Fm I and No I were recently measured with laser spectroscopy (Backe *et al.* (2005); Chhetri *et al.* (2018)).

Analyses of spectra of lanthanides and actinides are impeded by their sheer complexity and the large numbers of spectral lines and energy levels. For example, W.C. Martin worked for several tens of years at NBS and subsequently at NIST on the analysis of the Ce I spectrum. Some of his unpublished findings were included in the Handbook of Basic Atomic Spectroscopic Data (HBASD; Sansonetti & Martin (2005)), but the analysis was never brought to completion. For Nd I–II, an appendix to the Ph.D. thesis of J.-F. Wyart (Wyart (1973)) contains 9512 measured wavelengths. At his talk at this Symposium, Milan Ding of Imperial College, London, UK mentioned that their laboratory has precisely measured more than 20,000 lines of Nd I through Nd IV by using

Table 3. Popular databases containing atomic data on atomic wavelengths and radiative rates, which are online as of July 2022).

Database	**Z Range**	**Number of entries**	**Type of entries**	**Reference**
NIST ASD	1–99	291,639/122,655	lines/A-values	Kramida *et al.* (2021)
NIST Handbook (HBASD)	1–99	≈12,000	lines, many with A-values	Sansonetti & Martin (2005)
CHIANTI	1–30	1,954,916	transitions with A-values	Del Zanna *et al.* (2022)
AtomDB	1–30	99,510,189	transitions with A-values	Foster *et al.* (2022)
P. van Hoof's Atomic Line List	1–36	1,720,000	transitions, many with A-values	van Hoof (2010)
R.L. Kurucz's Atoms	1–53	2.3×10^6	transitions with A-values	Kurucz (2022)
Kelly's Line List	1–36	≈100,000	lines	Esmond & Smith (2008)
Spectr-W3	1–102	371,906	lines, many with A-values	Faenov *et al.* (2021)
CAMDB	1–95	$> 2,000,000$	transitions, many with A-values	Wu *et al.* (2022)
TOPBASE/ TIPBASE	1–26	1,715,706	f-values	Badnell *et al.* (2008)
VALD3	1–92	1,175,829	transitions with f-values	Ryabchikova *et al.* (2022)
DREAM	57–71	72,707	transitions with A-values	Quinet *et al.* (2020)
DESIRE	73–77	11,624	transitions with A-values	Fivet *et al.* (2020)
ACTINIDES	89–99	3600	lines	Blaise & Wyart (2006)
Splatalogue	1–8	53/5,800,000	lines (atoms/ molecules)	Remijan *et al.* (2020)
BRASS	1–92	82,337	lines with log gf-values	Lobel *et al.* (2019)
ISESA Grotrian	1–102	195,542/57,821	lines/A-values	Kazakov *et al.* (2021)

a Fourier transform spectrometer, and these spectra are currently being analyzed. This line list must be merged with Wyart's to provide a complete description of the first two neodymium spectra. For Pu I–II, a rather old report of Argonne National Laboratory contains 30,789 lines, only half of which were classified as transitions between pairs of levels (Blaise *et al.* (1984), Blaise *et al.* (1986)). To digitize and analyze such huge line lists is an enormous undertaking. Other lanthanide and actinide spectra are similarly complex and are impossible to be critically analyzed by a single team of workers. In addition to precise wavelengths and energy levels, transition probabilities of these spectra also need to be critically compiled from more than 500 papers published between 1960 and 2022 (Kramida & Fuhr (2010b)).

7.3. *Challenges specific to the Internet age*

As mentioned in Section 5, several online databases containing atomic data have appeared since the first release of NIST ASD in 1995. A brief list of the most popular of them is given in Table 3 with a very approximate description of their content.

The terms used in the 'Type of entries' column of Table 3 have meanings restricted to the context of this Table. 'Lines' means measured wavelengths of observed spectral lines, which may or may not be supplemented by classifications of lower and upper levels of the corresponding transitions. 'A-values and 'f-values' are two faces of the same quantity in the forms of transition probability (a.k.a. Einstein A-coefficient) and oscillator strength, respectively. 'Transitions' means Ritz wavelengths of specified electronic transitions, i.e., wavelengths calculated from the corresponding energy levels. Those energy levels may be experimental (i.e., determined from observed wavelengths) or theoretical. Wherever possible, the counts of transitions in the Table have been restricted to those determined from experimental energy levels. It was not possible in the case of the CAMDB database. Data for transitions involving theoretical energy levels usually have very low accuracy, and their use is limited. A large part of VALD3 data are derived from Kurucz's line lists.

In 2017, Pakhomov *et al.* (2017) wrote that VALD3 contains about 1.2 million accurate wavelengths and more than 250 million transitions with predicted parameters. Thus, Kurucz's Atoms database expands at a rapid pace, and so are many other databases listed in the Table. Information about the content of this database was obtained from the files in the `http://kurucz.harvard.edu/linelists/gfnew/` directory dated October 17, 2017. The present-day numbers may be significantly larger. Spectr-W3 and CAMDB collect and display data from multiple sources, so they may return multiple results for the same atomic transition or spectral line. It is difficult to estimate how many unique atomic transitions are contained in these databases. Of the total number of atomic transitions specified for CAMDB ($> 2,000,000$), most are theoretical data from recent accurate calculations, such as Wang *et al.* (2016). Although the authors of these calculations claimed "spectroscopic accuracy," in fact, a near-spectroscopic accuracy was achieved only for a small number of short-wavelength transitions, while wavelengths of the long-wavelength transitions are very inaccurate. In addition, many of these theoretical transitions are duplicated in terms of wavelength, since CAMDB indiscriminately included calculated transitions of all types considered in the source papers (e.g., E1 and M2), even though most of M2 transition rates are negligibly small. It is likely that the number of transitions with accurate experimental wavelengths in CAMDB is less than 500,000. The ISESA Grotrian database was described in Kazakov *et al.* (2017), but has significantly expanded since then.

None of the databases listed in Table 3, except NIST ASD, provide uncertainties for any of the physical quantities they contain. This is, in fact, legacy of the age of printed papers: page widths and volume of the articles were limited and did not allow the authors to include uncertainties for each measured wavelength. This was true, e.g., for all data published in CMS's compilations. Nowadays, tables can be published in electronic form as supplementary data, and their widths are unlimited. Nevertheless, many of the modern researches still follow the old traditions and publish their observational data without detailed information about uncertainties, which is a practice that must be eradicated completely. The situation is even worse for theoretical data. Although the NIST methodology for estimation of uncertainties of experimental and theoretical data was published already in 2013 (Kramida (2013)), most theorists are reluctant to use it; they do not provide estimates of uncertainties for each calculated wavelength and transition rate. This must change, since it is crucial to know the uncertainties for correct derivation of many physical quantities (e.g., the Hubble constant; see Section 6). The first versions of NIST ASD also did not contain explicit information about uncertainties. For wavelengths and energy levels, the uncertainties could be roughly estimated as "between 2 and 25 in the units of the last significant figure of the value." However, this is too imprecise for many purposes. Thus, in 2006 the NIST ASD team started the work on re-evaluation of archival data; this work included estimation of all uncertainties. By 2017, about half of the energy-level and wavelength data in the NIST ASD already had their uncertainties estimated, and the Web interface was modified to display these uncertainties (if available) in ASD version 5.5 released in that year. Nowadays, all new additions to ASD have measurement uncertainties specified for each wavelength and energy level. Uncertainties of the Ritz wavelengths are also estimated, stored, and displayed to the users. A similar work should be done for the content of all other atomic databases. This can be considered a task specific to the Internet age, since it was practically impossible to do before the birth of the WWW in the mid-1990s.

Each of the databases listed in Table 3 was designed for a specific purpose and targets a certain set of users. Many of them, such as CHIANTI, BRASS, AtomDB, and VALD3 target specifically the astrophysical community. CHIANTI and AtomDB include data on collisional rates and programming tools for modeling of absorption or emission spectra of plasmas typical for astrophysical environments. Many of the listed resources (HBASD, Kurucz's Atoms, DREAM, DESIRE, and ACTINIDES) are not really "databases" in the modern technical meaning of this term but are collections of static documents linked by a web interface and displayed in a web browser. Nevertheless, they all contain large numbers of fundamental atomic data that have applications in a wide range of areas not restricted by the specifics of their design. Thus, a universal data retrieval tool that could query many online databases and return the results in the same format is highly desirable. Such a tool would enable programmatic access to online databases, which would facilitate a better operation of computer codes for modeling of astrophysical and laboratory spectra.

The first step in this direction was made in 2009, when the Virtual Atomic and Molecular Data Centre (VAMDC) was initiated (Rixon *et al.* (2011)). The latest review of the status of this ongoing project was given by Albert *et al.* (2020). That paper listed 38 atomic and molecular databases connected to a common portal (VAMDC Portal). At present, the home page of this portal says that there are 41 databases connected to it. This undertaking was enabled by the development of a cross-database data exchange language, XSAMS (XML Schema for Atoms, Molecules and Solids; see `https://www-amdis.iaea.org/xsams/`). Members of the NIST ASG (most prominently, Yuri Ralchenko) were actively involved in development of this schema.

There still are many imperfections in XSAMS and in the functionality of the VAMDC Portal. Furthermore, the Portal is oriented towards a human user interactively building and running search queries. Automation of queries from computer codes is another challenge that needs to be worked out. Nonetheless, the pioneering work of the VAMDC Consortium has mapped a route for the future work and already established the key elements necessary for the future seamless integration of diverse atomic databases and modeling codes. The most important of these key elements are the data-exchange language (XSAMS) and the semantic layers with data dictionaries provided by specialized software for each data repository (Albert *et al.* (2020)).

8. Atomic spectroscopy databases at NIST

Physical Measurement Laboratory (PML) of NIST maintains and disseminates several online atomic-spectroscopy databases listed on its website,† which is referred to as PML-ADB further below. The NIST ASD (Kramida *et al.* (2021)) is listed there along with several separate entries that are actually parts of ASD, such as Laser Induced Breakdown Spectroscopy (LIBS) (`https://physics.nist.gov/libs`), Ground Levels and Ionization Energies (`https://physics.nist.gov/PhysRefData/ASD/ionEnergy.html`), and Atomic Spectra Bibliographic Databases (`https://physics.nist.gov/asbib`). Some atomic databases developed earlier by the NIST ASG, such as the Chandra database (see Ralchenko (2006a)), have already been completely integrated in ASD and discontinued as separate services. HBASD (Sansonetti & Martin (2005)), originally published on paper and as an e-book in 2005, continues to be distributed as a separate online database, although its content largely overlaps with ASD. One of the goals of the NIST ASD team is to completely eliminate data duplication in multiple databases, incorporate all content of HBASD into ASD, and discontinue HBASD as a separate online product. However, this task is impeded by the presence of data from unpublished (and unfinished) work for some spectra in HBASD, e.g., for Ce I, Tb I-II, Er I-II, as well as for all actinide spectra from Pa to Es. Some of these data are more accurate than all other published data, but they are incomplete, as Sansonetti and Martin (Sansonetti & Martin (2005)) have included only a few lowest energy levels

---

† `https://www.nist.gov/pml/atomic-spectroscopy-databases`

and a few strongest lines in their compilation. Inclusion of these data in ASD requires a complete re-analysis of all published data on these spectra, which is a daunting task.

Other databases listed on the PML-ADB page include Energy Levels of Hydrogen and Deuterium (Jentschura *et al.* (2005)), Ultraviolet Spectrum of Platinum Lamp (Sansonetti *et al.* (2003)), Spectrum of Th-Ar Hollow Cathode Lamps (Nave *et al.* (2008)), X-Ray Transition Energies Database (Deslattes *et al.* (2005)), SAHA Plasma Population Kinetics Modeling Database (Ralchenko (2006b)), and the recently added NIST-LANL Lanthanide Opacity Database (Olsen *et al.* (2022)). In addition to the databases, PML-ADB contains a link to an online plasma-modeling tool, collisional-radiative code FLYCHK (Chung *et al.* (2005)). Descriptions of all these resources are given on PML-ADB, as well as on their home pages, so there is no need to repeat them here. The NIST-LANL Lanthanide Opacity Database was described in detail by Yuri Ralchenko in his talk at this Symposium (Ralchenko (2022)).

9. Conclusions

As explained in this article, the work of Charlotte Moore Sitterly had and continues to have a great impact on fundamental and applied atomic physics. The standards of representation of atomic states and transitions in the literature and online databases stemmed largely from her work. She pioneered the activities on critical compilation of atomic energy levels and spectral lines. The atomic energy-level data she collected in her famous AEL reference books have migrated from paper into multiple online databases and continue to be actively used by atomic physicists, astronomers, and researchers in more than a hundred fields of fundamental and applied science. This is evidenced by the large numbers of citations in the literature, the rate of which began to grow fast after the introduction of online atomic databases. This is also indicated by statistics of user access to NIST ASD.

At the same time, most of the line lists compiled in CMS's Multiplet Tables have not been assimilated in online databases. This still needs to be done.

This article has outlined several urgent problems of the digital era of atomic spectroscopy.

- At present, no atomic spectroscopy database, except NIST ASD, provides uncertainties for the listed atomic parameters, such as energy levels, wavelengths, and radiative rates. Proper estimates of these uncertainties are necessary for correct modeling of plasma processes and for statistical analysis of large observational data sets. Even the NIST ASD provides dependable estimates of uncertainties for only half of its energy-level and wavelength data. The work on their evaluation must be continued. For radiative transition rates, most of the NIST ASD data do have uncertainty estimates. However, assessment of newly published data is greatly impeded by the lack of uncertainty estimates in most theoretical studies. The culture of theoretical research in atomic physics needs to be improved by adopting the published methodology of critical evaluation of data.
- Connectivity and interoperability of multiple online databases must be improved to allow for online computations, data comparisons, and analysis.
- Line lists and energy levels of lanthanides and actinides need a critical re-assessment. This is a huge work needing thousands of person-years. In general, the task of critical compilation of atomic data, which was "almost overwhelming" for CMS, is now impossibly large for a few people. It must be shared by all atomic spectroscopists.
- The paradigm of atomic spectroscopy research must change. Fragmentary studies are harmful to atomic spectroscopy, because they prevent rapid assimilation of improved data in the reference data sets. No single organization is capable of doing critical evaluation

of newly published studies at a rate comparable to that of new publications on atomic spectroscopy. Researchers must use the NIST methodology to critically re-evaluate all studies relevant to their projects.

References

Abbott, B.P., Abbott, R., Abbott, T.D., *et al.* 2017a, *ApJL*, 848, L12. doi:10.3847/2041-8213/aa91c9

Abbott, B.P., Abbott, R., Abbott, T.D., *et al.* 2017b, *PhRvL*, 119, 161101. doi:10.1103/PhysRevLett.119.161101

Albert, D., Antony, B.K., Ba, Y.A., *et al.* 2020, *Atoms*, 8, 76. doi:10.3390/atoms8040076

Bacher, R.F., & Goudsmit, S.A. 1931, Atomic Energy States – As Derived from the Analyses of Optical Spectra (New York: McGraw-Hill Book Co.), 562 pp.

Backe, H., A. Dretzke, St. Fritzsche, *et al.* 2005, Laser Spectroscopic Investigation of the Element Fermium ($Z = 100$), *Hyperfine Interact.*, 162, 3–14. doi:10.1007/s10751-005-9209-x

Badnell, N., Ballance, C., Bautista, M., Burke, P., Butler, K., Chen, G.-X., Delahaye, F., Del Zanna, G., Eissner, W., Fivet, V., Hudson, C., Liang, G.-Y., Mason, H., McLaughlin, B., Mendoza, C., Montenegro, M., Nahar, S., Oelgoetz, J., Palmeri, P., Pradhan, A., Quinet, P., Ramsbottom, C., Saraph, H., Scott, P., Storey, P., Wasson, I., Withoeft, M. & Zeippen, C. 2008, The Opacity Project – The Iron Project, online at: http://cdsweb.u-strasbg.fr/topbase/op.html (accessed 4 September 2022)

Blaise, J., Fred, M., & Gutmacher, R.G. 1984, The Atomic Spectrum of Plutonium, Argonne National Laboratory Report ANL-83-95, 612 pp. Online at: https://inis.iaea.org/search/search.aspx?orig_q=RN:16028008 (accessed on 7 September 2022)

Blaise, J., Fred, M., & Gutmacher, R.G. 1986, Term Analysis of the Spectrum of Neutral Plutonium, Pu I, *JOSAB*, 3, 403–418. doi:10.1364/JOSAB.3.000403

Blaise, J., & Wyart, J.-F. 2006, Selected Constants – Energy Levels and Atomic Spectra of Actinides, online at: http://www.lac.universite-paris-saclay.fr/Data/Database/ (accessed 8 September 2022)

Chhetri, P., D. Ackermann, H. Backe, *et al.* 2018, Precision Measurement of the First Ionization Potential of Nobelium, *PRL*, 120, 263003. doi:10.1103/PhysRevLett.120.263003

Chung, H.-K., Chen, M.H., Morgan, W.L., Ralchenko, Yu., & Lee, R.W. 2005, FLYCHK: Generalized population kinetics and spectral model for rapid spectroscopic analysis for all elements, *High Energy Density Phys.* 1, 3–12; online at: https://nlte.nist.gov/FLY/ (accessed 5 August 2020). doi:10.1016/j.hedp.2005.07.001

Clarivate Web of Science Database 2022, online at: https://www.webofscience.com/wos/woscc/basic-search (accessed on 5 September 2022)

Dalton, G. R., Dragoset, R.A., Fuhr, J.R., Kelleher, D.E., Kotochigova, S.A., Martin, W.C., Mohr, P.J., Musgrove, A., Olsen, K., Podobedova, L., Saloman, E.B., Sugar, J., Wiese, W.L., Stern Grant, C., Eichhorn, G., Kelly, R.L., Shirai, T., Azarov, V.I., Kramida, A.E., Ryabtsev, A.N., Blaise, J., & Wyart, J.F. 1998, in: Proc. Int. Conf. on Atomic and Molecular Data and Their Applications, NIST Spec. Publ. 926, W.L. Wiese and P.J. Mohr (eds.) (Washington, D.C.: U.S. Government Printing Office) 12–15; online at https://nvlpubs.nist.gov/nistpubs/Legacy/SP/nistspecialpublication926.pdf (accessed 4 September 2022)

Del Zanna, G., Young, P.R., Dere, K.P., *et al.* 2022, CHIANTI – An Atomic Database for Spectroscopic Diagnostics of Astrophysical Plasmas, Version 10.0.2 (George Mason University, USA; University of Michigan, USA; University of Cambridge, UK; NASA Goddard Space Flight Center, USA), online at: https://www.chiantidatabase.org/ (accessed 8 September 2022)

Deslattes, R.D., Kessler Jr., E.G., Indelicato, P., *et al.* 2005, X-ray Transition Energies, version 1.2 (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: https://physics.nist.gov/XrayTrans (accessed 13 September 2022)

DeVorkin, D. 1978, Charlotte Moore Sitterly, Interview on 15 June 1978 (College Park, MD, USA: Niels Bohr Library & Archives, American Institute of Physics).

Transcript is online at https://www.aip.org/history-programs/niels-bohr-library/oral-histories/4784 (accessed 6 September, 2022)

Ding, M. 2022, Kilonovae and the Cosmic Origin of r-Process Elements: Atomic Structure and Processes of Gold, Talk presented at IAUS371, International Astronomical Union General Assembly, 10 August 2022, Busan, Republic of Korea

Esmond, J.R., & Smith, P.L. 2008, Kelly (Cambridge, MA, USA: Harvard-Smithsonian Center for Astrophysics), online at: https://lweb.cfa.harvard.edu/ampcgi/kelly.pl (accessed 8 September 2022)

Faenov, A.Ya., Skobelev, I.Yu., Loboda, P.A., *et al.* 2021, Spectr-W3 Database on Spectroscopic Properties of Atoms and Ions (Russia: Russian Federal Nuclear Center – E.I. Zababakhin All-Russian Scientific Research Institute of Technical Physics, Joint Institute for High Temperatures of the Russian Academy of Sciences), online at: http://spectr-w3.snz.ru/index.phtml (accessed 8 September 2022)

Fivet, V., Quinet P., Palmeri P., *et al.* 2020, D.E.S.I.R.E. – DatabasE on SIxth Row Elements (Belgium: Mons University), online at: https://hosting.umons.ac.be/html/agif/databases/desire.html (accessed 9 September 2022)

Foster, A.R., Ji, L., Smith, R.K., *et al.* 2022, AtomDB – Atomic Data For Astrophysicists, Version 0.10.11 (Cambridge, MA, USA: Harvard-Smithsonian Center for Astrophysics), online at: http://www.atomdb.org/ (accessed 8 September 2022)

Fuhr, J.R., & Wiese, W.L. 1971, Bibliography on Atomic Transition Probabilities, July 1969 through June 1971; Natl. Bur. Stand. (U.S.), Spec. Publ. 320, Suppl. 1 (Washington, D.C.: U.S. Government Printing Office), 67 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-e647febaccfbf495ab09b180bc1f6c2e (accessed 4 September 2022)

Fuhr, J.R., Wiese, W.L., & Roszman, L.J. 1972, Bibliography on Atomic Line Shapes and Shifts (1889 through March 1972); Natl. Bur. Stand. (U.S.), Spec. Publ. 366 (Washington, D.C.: U.S. Government Printing Office), 154 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-76f55cc039acddfb1b667b248d65821d (accessed 4 September 2022)

Fuhr, J.R., & Wiese, W.L. 1973, Bibliography on Atomic Transition Probabilities, July 1971 through June 1973; Natl. Bur. Stand. (U.S.), Spec. Publ. 320, Suppl. 2 (Washington, D.C.: U.S. Government Printing Office), 63 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-0e024d314a3d917630978dafe02bddf9 (accessed 4 September 2022)

Fuhr, J.R., Roszman, L.J., & Wiese, W.L. 1974, Bibliography on Atomic Line Shapes and Shifts (April 1972 through June 1973); Natl. Bur. Stand. (U.S.), Spec. Publ. 366, Suppl. 1 (Washington, D.C.: U.S. Government Printing Office), 64 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-dac1747a1be070fc847e4306bd0d8bc9 (accessed 4 September 2022)

Fuhr, J.R., Martin, G.A., & Specht, B.J. 1975, Bibliography on Atomic Line Shapes and Shifts (July 1973 through May 1975); Natl. Bur. Stand. (U.S.), Spec. Publ. 366, Suppl. 2 (Washington, D.C.: U.S. Government Printing Office), 75 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-922f28e69edd562adb080fdc4cd39b96 (accessed 4 September 2022)

Fuhr, J.R., Miller, B.J., & Martin, G.A. 1978a, Bibliography on Atomic Transition Probabilities (1914 through October 1977); Natl. Bur. Stand. (U.S.), Spec. Publ. 505 (Washington, D.C.: U.S. Government Printing Office), 283 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-d5f4704857d2f3b49051e62abd7855eb (accessed 4 September 2022)

Fuhr, J.R., Miller, B.J., & Martin, G.A. 1978, Bibliography on Atomic Line Shapes and Shifts (June 1975 through June 1978); Natl. Bur. Stand. (U.S.), Spec. Publ. 366, Suppl. 3 (Washington, D.C.: U.S. Government Printing Office), 83 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-db619857d95d09fcbea65ebb3f6bdf26 (accessed 4 September 2022)

Fuhr, J.R., & Lesage, A. 1993, Bibliography on Atomic Line Shapes and Shifts (July 1978 through March 1992); Natl. Bur. Stand. (U.S.), Spec. Publ. 366, Suppl. 4 (Washington, D.C.: U.S. Government Printing Office), 288 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-f9c674871d1c31b716243a5842f677be (accessed 4 September 2022)

Glennon, B.M., & Wiese, W.L. 1962, Bibliography on Atomic Transition Probabilities, *NBS Monograph 50* (Washington, D.C.: U.S. Government Printing Office), 42 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-c29576d6fcbe243a4b5de511dddd0bf3` (accessed 4 September 2022)

Glennon, B.M., & Wiese, W.L. 1966, Bibliography on Atomic Transition Probabilities, *Miscellaneous Publications of NBS, No. 278* (Washington, D.C.: U.S. Government Printing Office), 92 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-d6f15603b276271eab50d3a198ce70c5` (accessed 4 September 2022)

Glennon, B.M., & Wiese, W.L. 1968, Bibliography on Atomic Transition Probabilities: May 1966 through December 1967, *Miscellaneous Publications of NBS, No. 278, Suppl. 1* (Washington, D.C.: U.S. Government Printing Office), 43 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-b53e455e582ae3d938dece17958996cb` (accessed 4 September 2022)

Gopka, V.F., Yushchenko, A.V., Shavrina, A.V, *et al.* 2005, *IAUS* 224, 734–742. doi:10.1017/S174392130500966X

Hagan, L., & Martin, W.C. 1972, Bibliography on Atomic Energy Levels and Spectra, July 1968 through June 1971, *Natl. Bur. Stand. (U.S.), Spec. Publ., No. 363* (Washington, D.C.: U.S. Government Printing Office), 109 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-1ae03a8ed7da5b28ead6e4f3496b6ee5` (accessed 4 September 2022)

Hagan, L. 1977, Bibliography on Atomic Energy Levels and Spectra, July 1971 through June 1975, *Natl. Bur. Stand. (U.S.), Spec. Publ., No. 363, Suppl. 1* (Washington, D.C.: U.S. Government Printing Office), 109 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-ccda39900c4383e6d5ae772c8765a802` (accessed 4 September 2022)

Haris, K., & Kramida, A. 2017, Critically Evaluated Spectral Data for Neutral Carbon (C I), *ApJS* 233, 16, doi:10.3847/1538-4365/aa86ab

Hu, J., Webb, J.K., Ayres, T.R., *et al.* 2021, Measuring the Fine-Structure Constant on a White Dwarf Surface; A Detailed Analysis of Fe V Absorption in G191-B2B, *MNRAS*, 500, 1466, doi:10.1093/mnras/staa3066

Jentschura, U.D., Kotochigova, S., LeBigot, E.O., Mohr, P.J., & Taylor, B.N. 2005, The Energy Levels of Hydrogen and Deuterium (version 2.1) (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: `https://physics.nist.gov/HDEL` (accesses 13 September 2022)

Kazakov, V.V., Kazakov, V.G., Kovalev, V.S., Meshkov, O.I., & Yatsenko, A.S. 2017, Electronic Structure of Atoms Information System: Current Status and Development Trends, *Optoelectron. Instrum. Data Proc.* 53, 136–144, doi:10.3103/S8756699017020054

Kazakov, V.V., Kazakov, V.G., Kovalev, V.S., Meshkov, O.I., & Yatsenko, A.S. 2021, Information System "Electronic Structure of Atoms" (Novosibirsk, Russia: Novosibirsk State University); online at: `http://grotrian.nsu.ru/en` (accessed 8 September 2022)

Kelly, R.L. 1987, Atomic and Ionic Spectrum Lines Below 2000 Angstroms: Hydrogen Through Krypton, J. Phys. Chem. Ref. Data 16, Suppl. 1 (Washington, DC: American Chemical Society), 1698 pp.

Kessler, K.G. 1988, Dr. Charlotte Moore Sitterly and the National Bureau of Standards, *JOSAB*, 5, 2043–2044

Kramida, A., Ryabtsev, A.N., Vedeneeva, G.V., & Kononov, E.Ya 1987, *BIBL – Bibliography Database on Atomic Spectra* (Troitsk, Russia: Institute of Spectroscopy, Russian Academy of Sciences); online at: `http://das101.isan.troitsk.ru/bibl.htm` (accessed 29 August 2022)

Kramida, A.E. 2007, Spectral Data for Tungsten Atoms and Ions, W I through W LXXIV, in: *Poster Papers of the 15th International Conference on Atomic Processes in Plasma (APIP-15)* (Gaithersburg, MD, USA: National Institute of Standards and Technology)

Kramida, A. 2010a, *Atomic Energy Levels and Spectra Bibliographic Database (Version 2.0)* (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: `https://physics.nist.gov/elevbib` (accessed 31 July 2020). doi:10.18434/T40K53

Kramida, A., & Fuhr, J.R. 2010b, *NIST Atomic Transition Probability Bibliographic Database (Version 9.0)* (Gaithersburg, MD, USA: National Institute of Standards and

Technology); online at: https://physics.nist.gov/fvalbib (accessed 31 July 2020). doi:10.18434/T46C7N

Kramida, A., & Fuhr, J.R. 2010c, *Atomic Line Broadening Bibliographic Database (Version 3.0)* (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: https://physics.nist.gov/linebrbib (accessed 31 July 2020). doi:10.18434/T4B59K

Kramida, A. 2011, Recent Developments in the NIST Atomic Databases, *AIP Conf. Proc.*, 1344, 81–95, doi:10.1063/1.3585808

Kramida, A. 2013, Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities, *Fusion Sci. Technol.*, 63, 313–323, doi:10.13182/FST13-A16437

Kramida, A. 2014, Using Databases for Data Analysis in Laser Spectroscopy, in: M. Baudelet (ed.), *Laser Spectroscopy for Sensing* (Cambridge, UK: Woodhead Publishing), Ch. 4, 102–124. doi:10.1533/9780857098733.1.102

Kramida, A., Ralchenko, Yu., Reader, J., & NIST ASD Team 2021, *NIST Atomic Spectra Database (Version 5.9)* (Gaithersburg, MD, USA: National Institute of Standards and Technology). Available online: https://physics.nist.gov/asd (accessed 31 July 2020). doi:10.18434/T4W30F

Kramida, A. 2022, Update of Atomic Data for the First Three Spectra of Actinium, *Atoms*, 10, 42. doi:10.3390/atoms10020042

Kramida, A., & Haris, K. 2022, Critically Evaluated Spectral Data for Singly Ionized Carbon (C II), *ApJS*, 260, 11, doi:10.3847/1538-4365/ac5401

Kurucz, R.L. 2022, Atomic and Molecular Spectra Database (Cambridge, MA, USA: Harvard-Smithsonian Center for Astrophysics), online at: http://kurucz.harvard.edu/ (accessed 4 September 2022)

Martin, W.C., Zalubas, R., & Hagan, L. 1978, Atomic Energy Levels – The Rare Earth Elements, Natl. Stand. Ref. Data Ser., NSRDS-NBS 60 (Washington, DC, USA: National Bureau of Standards), 422 pp.; online at: https://nvlpubs.nist.gov/nistpubs/Legacy/NSRDS/nbsnsrds60.pdf (accessed 7 September, 2022)

Lobel, A., Royer, P., Martayan, C., *et al.* 2019, The Belgian Repository of Fundamental Atomic Data and Stellar Spectra (BRASS), Atoms, 7, 105, doi:10.3390/atoms7040105. The database is available online at: http://brass.sdf.org/ (accessed 9 September 2022)

Martin, W.C. 1991, *Physics Today*, 44, 128–130

Martin, W.C., Dalton, G.R., Fuhr, J.R., Kelleher, D.E., Kramida, A., Mohr, P.J., Musgrove, A., Reader, J., Saloman, E.B., Sansonetti, C.J., Sugar, J., Wiersma, G.G., Wiese, W.L., Zucker, D., Blaise, J., Wyart, J.-F., Eichhorn, G., & Grant, C.S. 1995, NIST Laboratory Program on Atomic Spectroscopic Data for Astronomy, *Astron. Soc. Pac. Conf. Ser.*, 81, 597–601; online at http://www.aspbooks.org/a/volumes/article_details?paper_id=11089 (accessed 4 September 2022)

Martin, W.C., & Wiese, W.L. 1996, Atomic Spectroscopy, in: G.W.F. Drake (ed.), *Atomic, Molecular, and Optical Physics Handbook* (Woodbury, NY: AIP Press), p. 135–153. Online version of 2002 available at https://www.nist.gov/pml/atomic-spectroscopy-compendium-basic-ideas-notation-data-and-formulas (accessed 4 September 2022)

Miles, B.M., & Wiese, W.L. 1970, Bibliography on Atomic Transition Probabilities, January 1916 through June 1969, *NBS Special Publication 320* (Washington, D.C.: U.S. Government Printing Office), 103 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-eb48d25bef9982034369cc0c2cbd289e (accessed 4 September 2022)

Miller, B.J., Fuhr, J.R., & Martin, G.A. 1980, Bibliography on Atomic Transition Probabilities (November 1977 through March 1980), *Natl. Bur. Stand. (U.S.), Spec. Publ. 505, Suppl. 1*, (Washington, D.C.: U.S. Government Printing Office), 121 pp.; online at: https://www.govinfo.gov/app/details/GOVPUB-C13-fa39a1f7af6a3f993b1c573553304955 (accessed 4 September 2022)

Moore, C.E., & Russell, H.N. 1926, On the winged lines in the solar spectrum, *ApJ*, 63, 1–12

Moore, C.E. 1945, A Multiplet Table of Astrophysical Interest. Revised Edition. Part I – Table of Multiplets, Part II – Finding List of All Lines in the Table of Multiplets *Contrib. Princet. Univ. Obs.*, 20, 206 pp.

Moore, C.E. 1965, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – Si II, Si III, Si IV; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 1 (Washington, DC, USA: National Bureau of Standards), 35 pp., doi:10.6028/NBS.NSRDS.3sec1

Moore, C.E. 1967, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – Si I; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 2 (Washington, DC, USA: National Bureau of Standards), 35 pp., doi:10.6028/NBS.NSRDS.3sec2

Moore, C.E. 1968a, An Ultraviolet Multiplet Table, Sections 1 and 2, Hydrogen through Niobium (Reprint of NBS Circular 488, Sect. 1, 1950, and Sect. 2, 1952), *Nat. Bur. Stand. (U.S.) Circular 488, Sections 1 and 2* (Washington, DC, USA: National Bureau of Standards), 206 pp.

Moore, C.E. 1968b, An Ultraviolet Multiplet Table, Sections 3, 4, and 5, Molybdenum through Radium and Finding Lists (Reprint of NBS Circular 488, Sect. 3 through 5, 1962), *Nat. Bur. Stand. (U.S.) Circular 488, Sections 3, 4, and 5* (Washington, DC, USA: National Bureau of Standards), 204 pp.

Moore, C.E. 1968c, Bibliography on the Analyses of Optical Atomic Spectra, *Natl. Bur. Stand. (U.S.), Spec. Publ. 306, Sect. 1* (Washington, DC, USA: National Bureau of Standards), 80 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-9be8dee6faff93e34a5f9400cf5ee955` (accessed 4 September 2022)

Moore, C.E. 1969a, Bibliography on the Analyses of Optical Atomic Spectra, *Natl. Bur. Stand. (U.S.), Spec. Publ. 306, Sect. 2* (Washington, DC, USA: National Bureau of Standards), 80 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-b92934b569c8a1a04b11e99f12cf110e` (accessed 4 September 2022)

Moore, C.E. 1969b, Bibliography on the Analyses of Optical Atomic Spectra, *Natl. Bur. Stand. (U.S.), Spec. Publ. 306, Sect. 3* (Washington, DC, USA: National Bureau of Standards), 37 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-dbf501792ab238befc38e454773e683a` (accessed 4 September 2022)

Moore, C.E. 1969c, Bibliography on the Analyses of Optical Atomic Spectra, *Natl. Bur. Stand. (U.S.), Spec. Publ. 306, Sect. 4* (Washington, DC, USA: National Bureau of Standards), 48 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-ca0d2ba93161b122fe17f9332ff1feed` (accessed 4 September 2022)

Moore, C.E. 1970, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – C I, C II, C III, C IV, C V, C VI; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 3 (Washington, DC, USA: National Bureau of Standards), 73 pp., doi:10.6028/NBS.NSRDS.3sec3

Moore, C.E. 1971a, *Atomic Energy Levels as Derived from the Analysis of Optical Spectra – Hydrogen through Vanadium*; Nat. Stand. Ref. Data Ser., NSRDS-NBS 35, Vol. I (Reprint of NBS Circ. 467, Vol. I, 1949) (Washington, DC, USA: National Bureau of Standards), 359 pp., doi:10.6028/NBS.NSRDS.35v1

Moore, C.E. 1971b, *Atomic Energy Levels as Derived from the Analysis of Optical Spectra – Chromium through Niobium*; Nat. Stand. Ref. Data Ser., NSRDS-NBS 35, Vol. II (Reprint of NBS Circ. 467, Vol. II, 1952) (Washington, DC, USA: National Bureau of Standards), 230 pp., doi:10.6028/NBS.NSRDS.35v2

Moore, C.E. 1971c, *Atomic Energy Levels as Derived from the Analysis of Optical Spectra – Molybdenum through Lanthanum and Hafnium through Actinium*; Nat. Stand. Ref. Data Ser., NSRDS-NBS 35, Vol. III (Reprint of NBS Circ. 467, Vol. III, 1958) (Washington, DC, USA: National Bureau of Standards), 245 pp., doi:10.6028/NBS.NSRDS.35v3

Moore, C.E. 1971d, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – N IV, N V, N VI, N VII; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 4 (Washington, DC, USA: National Bureau of Standards), 46 pp., doi:10.6028/NBS.NSRDS.3sec4

Moore, C.E. 1972a, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – H I, D, T, Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 6 (Washington, DC, USA: National Bureau of Standards), 32 pp., doi:10.6028/NBS.NSRDS.3sec6

Moore, C.E. 1972b, A Multiplet Table of Astrophysical Interest, Revised Edition, Part I. Table of Multiplets, Part II. Finding List of All Lines in the Table of Multiplets; Nat. Stand. Ref.

Data Ser., NSRDS-NBS 40 (Washington, D.C.: U.S. Government Printing Office), 261 pp., doi:10.6028/NBS.NSRDS.40

Moore, C.E. 1975, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – N I, N II, N III; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 5 (Washington, DC, USA: National Bureau of Standards), 80 pp., doi:10.6028/NBS.NSRDS.3sec5

Moore, C.E. 1976, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – O I; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 7 (Washington, DC, USA: National Bureau of Standards), 33 pp., doi:10.6028/NBS.NSRDS.3sec7

Moore, C.E. 1979, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables – O VI, O VII, O VIII; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 8 (Washington, DC, USA: National Bureau of Standards), 31 pp., doi:10.6028/NBS.NSRDS.3sec8

Moore, C.E. 1980, Selected Tables of Atomic Spectra – A: Atomic Energy Levels – Second Edition, B: Multiplet Tables – O V; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 9 (Washington, DC, USA: National Bureau of Standards), 21 pp., doi:10.6028/NBS.NSRDS.3sec9

Moore, C.E. 1982, Selected Tables of Atomic Spectra – A: Atomic Energy Levels – Second Edition, B: Multiplet Table – O IV; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 10 (Washington, DC, USA: National Bureau of Standards), 21 pp., doi:10.6028/NBS.NSRDS.3sec10

Moore, C.E. 1985, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Table – O III; Nat. Stand. Ref. Data Ser., NSRDS-NBS 3, Sect. 11 (Washington, DC, USA: National Bureau of Standards), 33 pp., doi:10.6028/NBS.NSRDS.3sec11

Moore, C.E. 1993, Tables of Spectra of Hydrogen, Carbon, Nitrogen, and Oxygen Atoms and Ions, in: J.W. Gallagher (ed.), CRC Series in Evaluated Data in Atomic Physics (Boca Raton, FL: CRC Press), 339 pp.

Musgrove, A., & Zalubas, R. 1985, Bibliography on Atomic Energy Levels and Spectra, July 1970 through December 1983, *Natl. Bur. Stand. (U.S.), Spec. Publ., No. 363, Suppl. 3* (Washington, D.C.: U.S. Government Printing Office), 124 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-a2a52208e971b045b15566249246550b` (accessed 4 September 2022)

Nave, G., Sansonetti, C.J., & Kerber, F. 2008, Atlas of the Spectrum of a Th/Ar hollow cathode lamp in the region 691 nm to 5804 nm, version 1.1 (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: `https://physics.nist.gov/ThAr` (accessed 13 September 2022)

Olsen, K., Fontes, C.J., Fryer, C.L., Hungerford, A.L., Wollaeger, R.T., Korobkin, O., & Ralchenko, Yu. 2022, NIST-LANL Lanthanide Opacity Database, version 1.1 (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: `https://nlte.nist.gov/OPAC` (accessed 13 September 2022). doi: 10.18434/mds2-2375

Paschen, F. 1919, Das Spektrum des Neon, *Ann. Phys. (Leipzig)*, 365, 405–453

Pinho, A.M.M., & Martins, C.J.A.P. 2016, Updated constraints on spatial variations of the fine-structure constant, *PhLB*, 756, 121. doi:10.1016/j.physletb.2016.03.014

Pakhomov, Yu., Piskunov, N., & Ryabchikova, T. 2017, VALD3: Current Developments, in: *Stars: from Collapse to Collapse – ASP Conference Series, Vol. 510*, Yu.Yu. Balega, D.O. Kudryavtsev, I.I. Romanyuk, and I.A. Yakunin (eds.) (San Francisco, CA: Astron. Soc. of Pacific) 518–521; online at: `http://aspbooks.org/custom/publications/paper/510-0518.html` (accessed 10 September 2022)

Przybylski, A. 1961, HD 101065–a G0 Star with High Metal Content, *Nature*, 189, 739. doi:10.1038/189739a0

Quinet, P., Palmeri, P., Biémont, E. 2020, D.R.E.A.M. – Database on Rare Earths At Mons University (Belgium: Mons University), online at: `https://hosting.umons.ac.be/html/agif/databases/dream.html` (accessed 9 September 2022)

Ralchenko, Yu., Fuhr, J.F., Jou, F.-C., Kramida, A.E., Martin, W.C., Podobedova, L.I., Reader, J., Saloman, E.B., Sansonetti, J.E. & Wiese, W.L. 2005, New Generation of the NIST

Atomic Spectroscopic Databases, in: T. Kato, H. Funaba, & D. Kato (eds.), *Atomic and Molecular Data and their Applications, AIP Conference Proceedings 771* (Melville, NY: AIP Press), 276–285. doi:10.1063/1.1944716

Ralchenko, Yu. 2006a, A Guide to Internet Atomic Databases for Hot Plasmas, *JQSRT*, 99, 499–510. doi:10.1016/j.jqsrt.2005.05.040

Ralchenko, Yu. 2006b, NIST SAHA Plasma Kinetics Database, version 1.0 (Gaithersburg, MD, USA: National Institute of Standards and Technology), online at: `https://nlte.nist.gov/SAHA` (accessed 13 September 2022)

Ralchenko, Yu. 2022, NIST-LANL Lanthanide Opacity Database, Talk presented at IAUS371, International Astronomical Union General Assembly, 9 August 2022, Busan, Republic of Korea

Reader, J., Corliss, C.H., Wiese, W.L., & G. A. Martin 1980, Wavelengths and Transition Probabilities for Atoms and Atomic Ions, Part. I. Wavelengths, Part II. Transition Probabilities, Nat. Stand. Ref. Data Ser., NSRDS-NBS 68 (Washington, D.C.: U.S. Government Printing Office), 415 pp. doi:10.6028/NBS.NSRDS.68

Reader, J. 2006, Critical Compilation of Wavelengths and Energy Levels for Atoms and Atomic Ions, *J. Plasma Fusion Res. Series*, 7, 327–330

Redman, S.L., Nave, G., & Sansonetti, C.J. 2014, The Spectrum of Thorium from 250 nm to 5500 nm: Ritz Wavelengths and Optimized Energy Levels, *ApJS*, 211, 4. doi:10.1088/0067-0049/211/1/4

Remijan, A.J., Markwick-Kemper, A.J., Brogan, C., Turner, B., Williams, S. & Wootten, A. 2020, Splatalogue Database for Astronomical Spectroscopy, v. 3.0, online at: `https://splatalogue.online//` (accessed 4 September 2022)

Rixon, G., Dubernet, M.L., Piskunov, N., *et al.* 2011, VAMDC – The Virtual Atomic and Molecular Data Centre – A New Way to Disseminate Atomic and Molecular Data – VAMDC Level 1 Release, *AIP Conf. Proc.*, 1344, 107–115. doi:10.1063/1.3585810

Rubin, V.C. 2010, Charlotte Moore Sitterly, *Journal of Astronomical History and Heritage*, 13, 145-148; online at: `https://adsabs.harvard.edu/pdf/2010JAHH...13..145R`

Russell, H.N., & Saunders, F.A. 1925, New Regularities in the Spectra of the Alkaline Earths, *ApJ*, 61, 38–69

Ryabchikova, T.A., Piskunov, N.E., Pakhomov, Yu.V., *et al.* 2022, Vienna Atomic Line Database (VALD3), Version 3448 (Uppsala University, Sweden; Institute of Astronomy RAS, Moscow, Russia; University of Vienna, Austria), online at: `http://vald.astro.uu.se/~vald/php/vald.php` (accessed 8 September 2022)

Sansonetti, J.E., Reader, J., Sansonetti, C.J., Acquista, N., Sansonetti, A.M., & Dragoset, R.A. 2003, Atlas of the Spectrum of a Platinum/Neon Hollow-Cathode Lamp in the Region 1130–4330 Å, version 1.2 (Gaithersburg, MD, USA: Institute of Standards and Technology), online at: `https://physics.nist.gov/platinum` (accessed 13 September 2002)

Sansonetti, J.E., & Martin, W.C. 2005, Handbook of Basic Atomic Spectroscopic Data, *J. Phys. Chem. Ref. Data*, 34, 1559–2259; online at: `https://physics.nist.gov/handbook` (accessed 4 September 2022).

Suplee, C., & Kramida, A. 2012, Uses and Users of NIST's Atomic Spectra Database, *NIST News* Dec. 19; online at `https://www.nist.gov/news-events/news/2012/12/uses-and-users-nists-atomic-spectra-database` (accessed 4 September 2022)

VAMDC Consortium 2022, VAMDC Portal, online at: `https://portal.vamdc.org/vamdc_portal/home.seam` (accessed 10 September 2022)

van Hoof, P. (2010), The Atomic Line List v3.00b4, online at: `https://www.pa.uky.edu/~peter/newpage/` (accessed 4 September 2022)

Verner, D.A. 2000, Energy Levels, Wavelengths, Transition Probabilities, online at: `http://www.pa.uky.edu/~verner/lines.html` (accessed 4 September 2022)

Wang, K., Si, R., Dang, W., *et al.* 2016, Calculations with Spectroscopic Accuracy: Energies and Transition Rates in the Nitrogen Isoelectronic Sequence from Ar XII to Zn XXIV, *ApJS*, 223, 3. doi:10.3847/0067-0049/223/1/3

Webb, J.K., King, J.A., Murphy, M.T., Flambaum, V.V., *et al.* 2011, Indications of a Spatial Variation of the Fine Structure Constant, *PRL*, 107, 191101. doi:10.1103/PhysRevLett.107.191101

Wiese, W.L. 1996, The Critical Assessment of Atomic Oscillator Strengths, *Phys. Scr.*, T65, 188–191, doi:10.1088/0031-8949/1996/T65/028

Wilczynska, M.R., Webb, J.K., Bainbridge, M., *et al.* 2020, Four Direct Measurements of the Fine-Structure Constant 13 Billion Years Ago, *SciA*, 6, eaay9672. doi:10.1126/sciadv.aay9672

Wu, Y., Yan, J. *et al.* 2022, Atomic & Molecular Database (CAMDB) (Beijing, China: Institute of Applied Physics and Computational Mathematics), online at: `http://www.camdb.ac.cn/e/` (accessed 8 September 2022)

Wyart, J.-F. 1973, Classification des spectres d'arc et d'étincelle du dysprosium. Contribution a l'étude de configurations électroniques dans d'autres spectres des terres rares, Ph.D. Thesis, Univ. Paris-Sud, Orsay, France, 262 pp. Online at: http://www.lac.universite-paris-saclay.fr/Data/Theses/PDFTHESES/W/100-WYART%20J.F.%20(1973).pdf (accessed 8 September 2022)

Zalubas, R., & Albright, A. 1980, Bibliography on Atomic Energy Levels and Spectra, July 1975 through June 1979, *Natl. Bur. Stand. (U.S.), Spec. Publ., No. 363, Suppl. 2* (Washington, D.C.: U.S. Government Printing Office), 124 pp.; online at: `https://www.govinfo.gov/app/details/GOVPUB-C13-782c32b310e0b22bce571d625660a27c` (accessed 4 September 2022)

Appendix A: Citations to atomic data of CMS and NIST ASD

To better understand the impact of Charlotte More Sitterly and atomic data in general on modern science and technology, it is instructive to see what fields of science are citing CMS's AEL & MT publications and the NIST ASD. The distributions of fields of science citing AEL and MT are shown in Fig. 7.

AEL features about 15,000 citations in total, most of which come from fundamental sciences such as atomic physics and chemical physics, while only 2.4 % come from astronomy and astrophysics. In contrast, the MT publications, which are cited about 3000 times, are most popular among astronomers and astrophysicists, citations from this field of science constituting about 54 % of all citations of MT. In 1978, when asked what was the most significant of her research, CMS answered, "I think the 1945 Multiplet

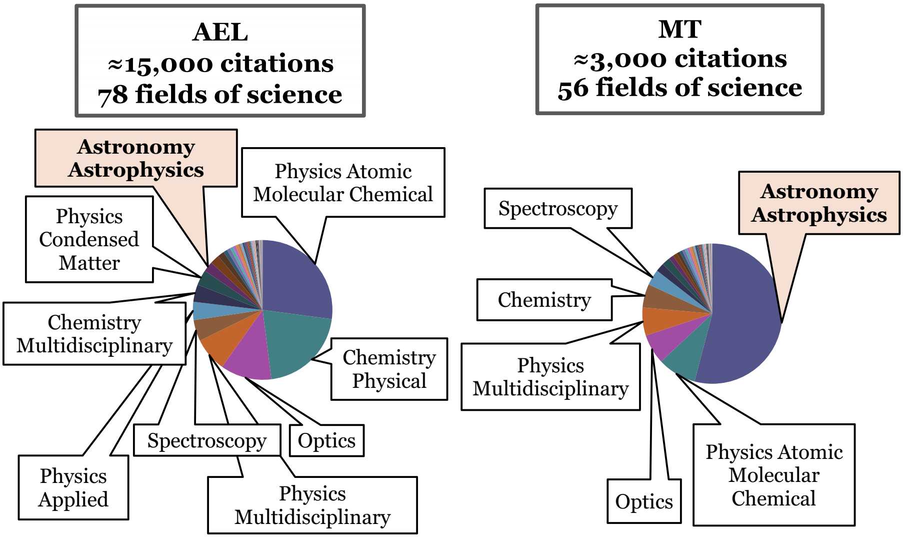


Figure 7. Fields of science citing CMS's AEL and MT publications from 1946 to 2022, from the Web of Science database (see references in the caption of Fig. 5).

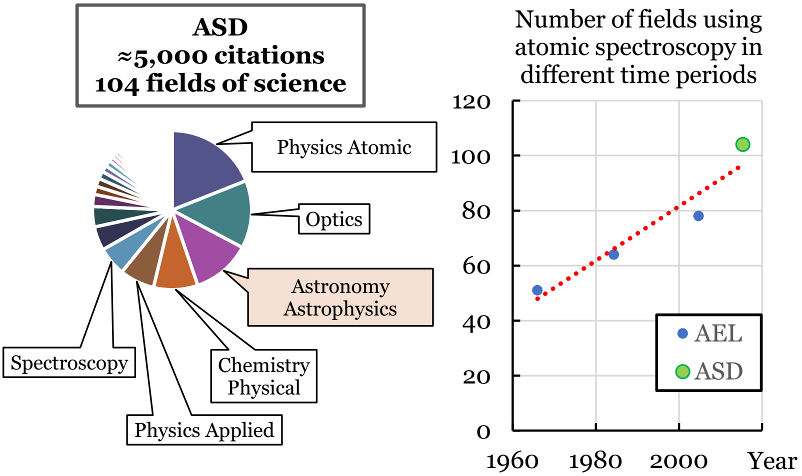


Figure 8. Left: Fields of science citing the NIST ASD from 1997 to 2022, from the Web of Science database (see references in the caption of Fig. 5). Right: Number of fields using atomic spectroscopy in different time periods (see text).

Table probably. It has had the most impact. All of the multiplet tables, and now my present series, I think, probably have had the most lasting influence on astrophysics and that has been my predominating interest. I have done those tables for the astronomers more than for the physicists" (DeVorkin (1978)). As Fig. 7 shows, she was correct from her own point of view: the MT was indeed most important for astronomy, which was her favorite subject. However, the AEL made a much deeper and broader impact on science in general and is cited five times more than MT. When looking at citations of the NIST ASD shown in the left panel of Fig. 8, it is impossible to discriminate what part of ASD is cited: energy levels or spectral lines. Thus, it is not surprising to see that the share of astronomy and astrophysics among all citations, 12 %, is somewhere in the middle between the fractions shown by Fig. 7 for AEL and MT.

The right panel of Fig. 8 shows the dynamics of counts of the fields of science citing reference publications on atomic spectroscopy. The data points in this plot were obtained by counting the number of fields of science in all citations of AEL in three periods of time: 1946–1972, 1973–1995, and 1996–2022 (small points), and citations of the NIST ASD in the period 1997–2022. Each count is attributed to a medium year of the period, which is a weighted average with weights equal to the citation rate per year shown in Fig. 5. Admittedly, this is not a strictly scientific plot, but it serves its purpose of showing a qualitative trend: applications of atomic spectroscopy broaden in time and now involve a very wide range of scientific areas.

For an interested reader, the counts of citations to AEL, MT, and ASD, obtained from the Web of Science database (Clarivate (2022)) in July 2022 are listed in Table 4 for the 113 fields of science involved.

Table 4. Counts of citations to AEL, MT, and ASD per field of science (from the Web of Science database, Clarivate (2022), as of July 2022).

WOS category	AEL	MT	ASD	WOS category	AEL	MT	ASD
Physics Atomic Molecular Chemical	6380	256	1470	Engineering Environmental	5		3
Optics	2792	197	1069	History Philosophy Of Science	2		3
Astronomy Astrophysics	558	1546	927	Materials Science Characterization Testing	2		3
Chemistry Physical	4924	155	698	Archaeology			2
Physics Applied	992	57	549	Biotechnology Applied Microbiology	1		2
Spectroscopy	1153	105	456	Computer Science Artificial Intelligence	1		2
Physics Multidisciplinary	1859	185	376	Computer Science Information Systems	6		2
Physics Fluids Plasmas	96	31	322	Computer Science Theory Methods	11	2	2
Materials Science Multidisciplinary	510	16	190	Engineering Marine			2
Instruments Instrumentation	122	28	129	Materials Science Composites			2
Physics Nuclear	152	15	128	Microbiology			2
Chemistry Multidisciplinary	946	19	120	Operations Research Management Science	1		2
Chemistry Analytical	140	21	104	Plant Sciences	1		2
Physics Condensed Matter	843	15	98	Public Environmental Occupational Health			2
Nuclear Science Technology	83	18	73	Robotics			2
Engineering Electrical Electronic	127	12	64	Telecommunications	5		2
Materials Science Coatings Films	51	2	61	Mathematical Computational Biology	2		1
Nanoscience Nanotechnology	42	2	52	Pharmacology Pharmacy	1		1
Multidisciplinary Sciences	193	55	51	Statistics Probability	1		1
Engineering Chemical	54	4	49	Toxicology	1		1
Thermodynamics	38	2	39	Mathematics		1	1
Engineering Mechanical	19	1	37	Agronomy			1
Energy Fuels	22	2	34	Anthropology			1
Geosciences Multidisciplinary	4	13	32	Art			1
Chemistry Inorganic Nuclear	360	5	31	Ecology			1
Engineering Aerospace	28	8	31	Engineering Ocean			1
Meteorology Atmospheric Sciences	5	12	31	Geography Physical			1
Physics Mathematical	29	7	31	Geology			1
Physics Particles Fields	85	6	30	Marine Freshwater Biology			1
Food Science Technology			28	Materials Science Biomaterials			1
Geochemistry Geophysics	9	9	27	Materials Science Paper Wood			1
Metallurgy Metallurgical Engineering	59	1	23	Materials Science Textiles			1
Quantum Science Technology	220	6	22	Medical Laboratory Technology			1
Biochemical Research Methods	36		21	Medicine Research Experimental			1
Environmental Sciences	6		20	Respiratory System			1
Biochemistry Molecular Biology	53	4	18	Transportation Science Technology			1
Engineering Manufacturing	4		17	Water Resources			1
Computer Science Interdisciplinary Applications	24	3	16	Microscopy	6		
Mathematics Interdisciplinary Applications	167	4	15	Biology	5		
Mechanics	22	4	14	Computer Science Hardware Architecture	4	2	
Polymer Science	5	1	14	Computer Science Software Engineering	4	2	

Table 4. Continued.

WOS category	AEL	MT	ASD
Radiology Nuclear Medicine Medical Imaging	3	1	13
Chemistry Applied	12	1	12
Biophysics	15	1	10
Education Scientific Disciplines	42	1	9
Mineralogy	4	1	7
Soil Science			7
Automation Control Systems	1		6
Engineering Industrial	1		6
Imaging Science Photographic Technology	3		6
Mining Mineral Processing	1		6
Remote Sensing		2	6
Crystallography	31	3	5
Materials Science Ceramics	19		5
Mathematics Applied	7	2	5
Oceanography		1	5
Acoustics	1		4
Construction Building Technology			4
Electrochemistry	12		4
Engineering Biomedical		1	4
Green Sustainable Science Technology			4
Nutrition Dietetics			4
Chemistry Organic	79	1	3
Endocrinology Metabolism			3
Engineering Civil			3
Social Sciences Interdisciplinary	3	2	
Engineering Geological	1		
Engineering Petroleum	1		
Information Science Library Science	1	1	
Agriculture Multidisciplinary		1	