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On Atomic Physics Data for Stellar Atmospheres Research

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Abstract. I extend the discussion of Cowley, Adelman & Bord (2003) in regard to the sources of atomic data especially as concerns line identifications and gf values.

Key words. Atomic data – Line identification

1. Introduction

For IAU Symposium No. 210, Modelling of Stellar Atmospheres, Charles R. Cowley, Donald J. Bord, and I presented a paper on the same general topic as this paper (Cowley et al. 2003). Here I revisit the sources of atomic data section. I am doing this as a user of atomic data rather than of a producer of atomic data. Glenn Wahlgren (Wahlgren 2005) discusses some additional subjects.

Some thirty years ago, I had the pleasure of meeting Dr. Charlotte Moore Sitterly who was one of the most prolific organizers of atomic data. She was both an atomic and an astrophysical spectroscopist. Her data compilations, which often involved critical evaluation, were done using 3 inch by 5 inch note cards. She was not an exponent of computers in part as she rightly feared they would make possible access to a large amount of data whose quality was unknown to the user. Dr. Sitterly believed that the data users should read the original papers and become sufficiently expert to evaluate the variety of data sources. Unfortunately today many atomic data users are not experts on the various experimental techniques used to measure atomic data of use in stellar atmospheres. Furthermore most of us are not sufficiently grounded in the theoretical techniques used to predict similar values to be able to evaluate them.

Two approaches that stellar astronomers often use are 1) to trust critical evaluators and 2) to learn something of how the experts evaluate the quality of research performed at various institutions and by the active workers in the field. The critical evaluation of atomic data requires being familiar with a variety of techniques and understanding their strengths and weaknesses. It is a vital service to the scientific community at large. When different sources provide discrepant values one especially needs to consider the errors in the values provided. This is often quite difficult for the non-expert. and the critical evaluators act as the proxies for data users. Even if you trust the critical evaluators, it is still an excellent idea to learn something of their methodology and once in a while to read atomic spectroscopy papers of interest to you. You can often gain information about

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Table 1. Recent Sources of Atomic Line Identification Lists

Be II	Jupen, C., Meigs, A, von Hellermann, M,, Beringer, M., Granzen, A., & Martinson, I. 2001, Phys. Scripta, 64, 563 [EA, 2223-5441]
Be III	Jupen, C., Meigs, A, von Hellermann, M,, Morsi, H. W., et al. 2001, Phys. Scripta, 64, 566 [EA, 81-6142]
Ne IV	Kramida, A. E., Bastin, T., Biemont, E., Dumont, P.-D., & Garnir, H.-P. 1999, Eur. Phys. J. D, 7, 525 [EA, 140-4726]
Ne V	Kramida, A. E., Bastin, T., Biemont, E., Dumont, P.-D., & Garnir, H.-P. 1999, Eur. Phys. J. D, 7, 547 [EA, 107-243175]
S VII	Jupen, J., Engstrom, L. 2002, Phys. Scripta, 66, 140 [EA, 46-3890]
Ar I	Whaling, W., Anderson, W. H. C., Carle, M. T., Brault, J. W., & Zarem, H. A. 2002, JRNIST, 107, 149 [AW, 332- 5865]
Fe V	Ararov, V. I., Tchang-Brillet, W.-U L., Wyart, J.-F., Launay, F., & Beharrous, M. 2001, Phys.Scripta, 63, 438 [EA, 647-1185]
Ga II	Karlsson, H., & Litzen, U. 2000, J. Phys. B 33, 2929 [AW, I 2607-2692, II 2090-7579]
Nb II	Ryabtsev, A. N., Churilov, S. S., & Litzen, U. 2002, Phys. Scripta, 62, 368 [EA, 1588-4894]
Mo II	Nilsson, H., & Pickering, J. C. 2003, Phys. Scripta, 67, 223 [EA. 1500-7000]
Ru II	Karlsson, H., Joueizadeh, A., & Johansson, S. 2002, Phys. Scripta, 66, 238 [AW, 1875-4373]
Pd II	Litzen, U., Lundberg, H., & Tchang-Brillet, W.-U L.. 2001, Phys. Scripta, 64, 63 [EA, 1044-2000, 2117-3122, 8184-40036]
Ag I	Pickering, J. C., & Vilio,V. 2001, Eur. Phys. J., D, 13, 181 [AW, 2061-8274]
Ag II	Kalus, G., Litzen, U., Launay, F., Tchang-Brillet, W.-U L. 2002, Phys. Scripta, 65, 46 [RA, 943-8404]
In I, II	Karlsson, H., & Litzen, U. 2001, J. Phys. B 34, 4475 [RA , I 2775-3052, II 1586-7841]
I III	Tauheed, A., & Joshni, Y. N., Naz, A. 2004, Phys. Scripta, 69, 289 [EA, 453-1124]
I IV	Tauheed, A., & Joshni, Y. N., Naz, A. 2004, Phys. Scripta, 69, 283 [EA, 364-536]
Pr II	Ivarsson, S., Litzen, U., & Wahlgren, G. M. 2001, Phys. Scripta, 64, 455 [AW, 3877-5382]
Dy I, II	Nave, G., & Griesmann, U. 2000, Phys. Scripta, 62, 463 [CL, I 3297-16549, II 2281-6126]
Ta II	Eriksson, M., Litzen, U., Wahlgren, G. M., & Leckrone, D. S. 2002, Phys. Scripta, 65, 480 [ID, 1988-4236]
Ta III	Azarov, V. I., Tchang-Brillet, W.-U L.,Wyart, J.-F., & Meijer, F. G. 2003, Phys. Scripta, 67, 190 [A, 1099-3944]
Hg II	Sansonetti, C. J., & Reader, J. 2001, Phys. Scripta, 63, 219 [RA, 558-9760]
Bi I/II/III	Wahlgren, G. W., Brage, T., Brandt. J. C., et al. 2001, ApJ.. 551. 520 [ID, I 1685-3113, II 1058-3118, III 1051-2857]
Bi II	Dolk, L., Litzen, U., & Wahlgren, G. M. 2002, A&A, 388, 692 [RA, 1436-6910]

Notes: A=Analysis, AW = accurate wavelengths, CL = classified lines, EA = extended analysis, ID = Identified Lines, RA = revised analysis whose work is the most trusted by reading the critical evaluation papers and by talking with colleagues who are active in the field.

I also strongly suggest that all users of atomic data meet the producers and let them know which of their studies you have used in your research. Many of them are very willing to help you if they can and eager to learn how their work benefited you. If you are a member of the International Astronomical Union, please consider joining Commission 14, Atomic and Molecular Data.

2. Databases

Yuri Ralchenko (2005) of NIST has kindly provided a description of the new NIST Atomic Spectra Database which can be found at: http://physics.nist.gov/PhysRefData/ASD/index.html. Version 3.0 contains critically evaluated NIST data for radiative transitions in atomic species. It contains data for the observed transitions of 99 elements and energy levels of 57 elements and is an excellent starting place for this kind of material. Additional NIST databases and papers can be accessed via http://physics.nist.gov/PhysRefData/contents.html.

Another site that may provide some useful data is that of the International Atomic Energy Agency (IAEA) Nuclear Data Section/Atomic and Molecular Data Unit (http://www-amdis.iaea.org). This site has Databases on Atomic and Molecular Data for Fusion, GENIE (General Internet Search Engine) which searches for spectral and collisional atomic data for fusion and atomic physics research as well as provides access to two Chinese databases, and four online computing portals including the Los Alamos atomic physics codes. The IAEA publishes an ”International Bulletin on Atomic and Molecular Data for Fusion”.

If you require recent information on the Rare Earth Elements, an excellent source is the Database on Rare Earth Elements at Mons University (DREAM) of E. Biemont, P. Palmeri, and P. Quinet (http://w3.umh.ac.be/~astro/dream.shtml) which consists of materials from the papers of the three organizers and their collaborators.

A combination of data from these sources, from VALD (Kupka et al. 2000), and from the Kurucz database (Kurucz 2005) provide the basis for an encouraging synthesis of the atomic and some molecular features in at least the optical region of most stars. I prefer the NIST critical compilations, then the more recently published sources recommended by the NIST critical compilers as those they will use for their next such efforts, high quality theoretical compilations, VALD, and then whatever I can find. Such an order reflects my prejudices and experience. Different atomic and stellar astrophysicists make their own choices due to their personal experiences.

3. Gf Values and Line Broadening

From the introductions to the forthcoming NIST compilations of Fe I and Fe II gf values (Fuhr & Wiese 2005) I learned why there have been important recent improvement of gf values. For previous compilations of Fe I, the emission measurements used stabilized arcs that were later shown to be in a state of partial local thermodynamic equilibrium. Such experiments provided relative values that were subsequently normalized to a few available lifetime data. They have been now largely superceded by research that uses simpler emission branching ratio measurements in combination with numerous especially determined lifetimes. The sources are inductively coupled plasmas of hollow cathodes of lower density. LTE is neither assumed or required. Measurements of specific upper energy levels yield the branching ratios or branching fractions. Lifetimes are found for all pertinent levels to place the branching ratio data on an absolute scale.

For Fe II the number of lines and the quality of the gf values also have been improved. In the 1988 compilation (Fuhr et al. 1988) experimental data by Whaling were the best. These were found by a combination of accurate emission branching fractions generated with a hollow cathode and measured with a Fourier Transform Spectrometer (FTS) and lifetimes obtained with high-quality laser induced fluorescence (LIF) measurements. In the new compilation about 2/3 of the compiled data were derived using this approach.

Not all atomic transitions can be described by pure L-S coupling. For some atomic species j-j coupling and intermediate coupling are better approximations to what is observed. Many transitions are between terms that have multiple parentage.

In some cases, the theoretical gf values are preferred to the experimental values by the NIST evaluators. I find it very educational to learn how these calculations are performed. Over the years Kurucz's theoretical gf value results have improved as new atomic levels have been found and the upper levels from which lines of interest arise have become better embedded in the system as a whole. Kurucz provides line damping constants which most other sources do not. His data is often the only source of gf values sufficiently good for use in elemental abundance analyses.

The radiative lifetime of a level is found from the transition probabilities for all possible downward radiative transitions from that level. As the ground state has an infinite lifetime, it has a zero radiative width. For resonance lines the primary decay path for the upper level is the resonance line itself. Thus the radiative width of the level and line is essentially the inverse of the transition probability. When the transition probabilities are available for all the decays from a level, use them rather than any simple formula to calculate the radiative widths.

Collisional broadening (Stark widths) depend on collisional transitions. Some calculations are available especially by Dimitrijevic and his associates (see e.g., Dimitrijevic & Sahal-Brechot 2004, Dimitrijevic et al. 2004). For the van der Waals coefficients Kurucz's approximations should suffice.

4. Line Identifications

When performing stellar line identifications, studies of sharp-lined stars are quite useful. But often the identifications still will be incomplete as the wavelength ranges do not completely coincide or as the elemental abundances values are not the same. In this case one could start with a Multiplet Table of Astrophysical Interest (Moore 1945) and then for certain atomic species to its supplements (Moore 1993). A finding list of the first 10 sections was produced by Adelman et al. (1993). Line lists are also included in the NIST Atomic Spectra Database. Recent sources are given in Adelman (2001) and references therein. Previous papers of this series contain information on older papers. A list of subsequent references is given in Table 1. Another good source to begin a search are the triannual reports of IAU Commission 14.

One can also synthesize spectra using SYNTHE (Kurucz & Avrett 1981) and similar programs. This is a quite useful method to identify lines without identifications after one has performed an initial line identification study so that the line strengths are approximately correct for as many species as possible.

The ease with which stellar spectra now can be synthesized definitely reduces the value of the classical stellar line lists that provide wavelengths, equivalent widths, and the author's best guess at the identification(s). Still they can be valuable especially when they are available in digital form and produced using high dispersion high signal-to-noise spectra. Some are in the literature, others in the literature and on home pages e.g., for Deneb (Albayrak et al. 2003) see http://www.brandonu.ca/Physics/gulliver/atlases.html, others are on astronomers home pages, e.g., Charles R. Cowley has several line lists on his home page (http://www.astro.lsa.umich.edu/users/cowley and still others are available by asking the person who performed the study. I have provided such lists when requested. Features that lack oscillator strengths cannot be synthesized, but still they will appears in the stellar line lists. Castelli & Hubrig's (2004) study of HR 7143 is an example of the power of synthesis (see also Castelli's home page, http://wwwuser.oat.ts.astro.it/castelli). However, plots of the synthetic and observed spectra may not be as convenient as line lists. Their identifications may not be in digitized form and global searches for all the lines of an atomic species, such as Mn II, may not be easy to do from the plots.

If you need information on diatomic molecules, you might consult RADEN (The data bank on RADiative and Energy parameters for diatomic molecules) at http://www.elech.chem.msu.ru/raden/index.htm. It has two parts, a reference information system and a recommended data system. This well regarded effort is produced at the Department of Chemistry of Moscow State University.

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