NRC Research Press

ARTICLE

Including all the lines: data releases for spectra and opacities[1]

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Abstract: I present a progress report on including all the lines in the line lists, including all the lines in the opacities, and including all the lines in the model atmosphere and spectrum synthesis calculations. The increased opacity will improve stellar atmosphere, pulsation, stellar interior, asteroseismology, nova, supernova, and other radiation-hydrodynamics calculations. At present I have produced atomic line data for computing opacities for 544 million lines for elements up through Zn. Of these, 2.11 million lines are between known energy levels so have good wavelengths for computing spectra. Work is continuing on heavier elements. I also report on using stellar spectra as the laboratory source for extending analyses to higher energy levels. Data for each ion and merged line lists are available on my website kurucz.harvard.edu.

Key words: atomic spectroscopy, molecular spectroscopy, oscillator strengths, opacity, stellar atmospheres.

Résumé : Je présente un rapport d'avancement sur l'inclusion de toutes les raies dans la liste des raies, incluant toutes les raies dans les opacités et incluant aussi toutes les raies dans le modèle d'atmosphère et les calculs de synthèse de spectre. L'opacité accrue va améliorer les calculs d'atmosphère stellaire, de pulsation, d'astroséismologie, de nova, de supernova et d'autres calculs mêlant radiation et hydrodynamique. J'ai maintenant produit des données de raies atomiques destinées au calcul d'opacité pour 544 millions de raies dans les éléments allant jusqu'au Zn. Parmi celles-ci, 2.11 millions de raies correspondent à des transitions entre niveaux connus et ont ainsi de bonnes longueurs d'onde pour les calculs spectraux. Le travail continue sur les éléments plus lourds. Je rapporte aussi l'utilisation de spectres stellaires comme source laboratoire pour étendre les analyses aux niveaux d'énergie plus élevée. Les données pour chaque ion et la liste augmentée de raies sont disponibles sur ma page web à kurucz.harvard.edu. [Traduit par la Rédaction]

Mots-clés : spectroscopie atomique, spectroscopie moléculaire, forces d'oscillateur, opacité, atmosphères stellaires.

1. Introduction

I described the "Including all the lines" project at ASOS 10 in 2011 [1]. I refer the reader to that paper for the many included tables and color figures that I will not repeat here. I also do not repeat the sections on my model atmosphere, spectrum synthesis, and opacity programs, and the section on high-quality atlases for use in verifying the line data. Here I quote the first two background sections from that paper and then report on the current status.

In 1965 I started collecting and computing atomic and molecular line data for computing opacities in model atmospheres and then for synthesizing spectra. I wanted to determine stellar effective temperatures, gravities, and abundances. I still want to.

For 23 years I put in more and more lines but I could never get a solar model to look right, to reproduce the observed energy distribution.

In 1988 I finally produced enough lines, I thought. I completed a semiempirical calculation of the first nine ions of the iron group elements using my versions of Cowan's atomic structure programs [2] and least-squares fitting to the compilation of laboratory energy levels by Sugar and Corliss [3]. There were data for 42 million lines that I combined with data for 1 million lines from my earlier list for lighter and heavier elements including all the data from the literature. In addition I had computed line lists for diatomic molecules including 15 million lines of H_2, CH, NH, OH, MgH, SiH, C_2, CN, CO, SiO, and TiO for a total of 58 million lines.

I tabulated 2 nm resolution opacity distribution functions from the line list for temperatures from 2000 to 200 000 K and for a range of pressures suitable for stellar atmospheres [4].

Using the opacity distribution functions I computed a theoretical solar model [5] with the solar effective temperature and gravity, the then current solar abundances from Anders and Grevesse [6], mixing-length-to-scale-height ratio $l/H = 1.25$, and constant microturbulent velocity 1.5 kms^{-1}. It generally matched the observed energy distribution from Neckel and Labs [7].

I computed thousands of model atmospheres that I distributed on magnetic tapes, then on CDs, and now on my web site, kurucz.harvard.edu. They made observers happy. However, agreement with low resolution observations of integrated properties does not imply correctness.

2. Problems

In 1988 the abundances were wrong, the microturbulent velocity was wrong, the convection was wrong, and the opacities were wrong.

Since 1965 the solar Fe abundance determination has varied by over a factor of 10. In 1988 the Fe abundance was 1.66 times larger than today. There was mixing-length convection with an exaggerated, constant microturbulent velocity. In the grids of models, the default microturbulent velocity was 2 kms^{-1}. My 1D models still have mixing-length convection, but now with a depth-dependent microturbulent velocity that scales with the convective velocity.

Received 31 October 2016. Accepted 28 November 2016.

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[1]This paper is part of a Special Issue on the 12th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas held at the Universidade de São Paulo on 4–7 July, 2016.

Table 1. Partial statistics for the semiempirical ion calculations completed thus far.

	Configurations		Levels		E1 lines		
Ion	Even	Odd	Even	Odd	Total	Good wl	Date
Li I	35	32	59	59	938	938	9 Feb 15
F I	48	46	997	962	131375	5461	17 Jan 15
F II	59	60	2026	2214	206549	9355	11 Jan 15
F III	64	60	2033	1851	389119	9835	29 Dec 14
F IV	61	61	1500	1480	342404	4413	18Oct16
F V	58	54	807	762	93392	3208	15 Oct 16
F VI	61	58	366	320	42842	3788	21 Oct 16
Ar I	52	53	405	396	49824	16649	2 Sep 11
Ar II	47	47	1001	1024	230953	17188	2 Sep 11
Ar III	48	48	1682	1790	419776	1881	2 Sep 11
Ar IV	33	34	1278	1111	409425	486	2 Aug 16
Ar V	61	61	1616	1638	446472	325	29 Jul 16
Ar VI	61	61	668	751	137526	327	5 Aug 16
Cr I	47	40	18842	18660	2751796	37147	22Jan16
Cr II	61	61	13767	15890	8683460	90613	27 Jan 16
Cr III	61	61	6560	7526	6436134	13150	22 Jul 14
Cr IV	61	61	2094	2318	1044865	2590	6 Sep 15
Cr V	61	61	509	636	109427	252	5 Sep 15
Cr VI	33	32	134	147	10125	357	17 Aug 15
Cr VII	32	33	245	253	121069	590	13 Aug 15
Cr VIII	56	52	1555	1281	729126	35	2 Apr 16
Cr IX	53	54	1453	1456	756558	80	9 Apr 16
Zn I	72	72	566	681	34135	6282	4 Jan 12
Zn II	61	61	926	1286	31563	968	13 Jan 12
Zn III	61	61	4303	5758	640536	12674	13 Jan 12
Zn IV	61	61	10252	11429	5715894	7214	12 Jun 16
Zn V	60	50	18353	19364	13806567	2544	16 Jun 16
Zn VI	44	39	18343	19517	21467731	1614	3 Jun 16
Zn VII	46	41	18208	19238	24491877	1498	24 Jun 16
Zn VIII	61	61	13706	15660	21677814	3	13 Jul 16
Zn IX	61	61	6560	7526	7226420	0	14 Jul 16
Y II	69	65	806	930	145597	7213	30 Sep 11

Three-dimensional models with cellular convection do not have microturbulent velocity at all, but use the Doppler shifts from the convective motions.

In 1988 the line opacity was underestimated because not enough lines were included in the line lists. High configurations up through n = 9 or 10 were not included in the calculation because of computer limitations and the lack of laboratory data. Thus the higher energy levels that produce series of lines that merge into ultraviolet (UV) continua were not included. Those levels also produce huge numbers of weaker lines in the visible and infrared regions that blend and fill in the spaces between the stronger lines. Also lines of heavier elements were not systematically included. And then the additional broadening from hyperfine and isotopic splitting was not included.

In 1988 the opacities were low but were balanced by high abundances that made the lines stronger and high microturbulent velocity that made the lines broader. Now the abundances, the convection, and the opacities are still wrong, but they have improved. I am concentrating on filling out the line lists.

3. Progress report

Table 1 shows partial statistics for the semiempirical calculations completed thus far: the ion name, the number of even and odd configurations, the number of even and odd energy levels, the total number of E1 lines saved, the number of lines with good wavelengths that connect known energy levels, and the date when the E1 calculation was completed. The whole table can be found on my website as /atoms/completed.txt. I have computed the first six ions up through K and the first nine or 10 ions for Ca through Zn. And also Sr I, Y I, and Y II. I have much work still ahead: the 4d group Sr–Cd, Ga–Y, In–Ba, lanthanides, heavy elements, and higher ions for the 3d group.

All of the previous work by Kurucz and Peytremann in 1975 [8] and by Kurucz in 1988 [2] has been replaced. There are an order of magnitude more lines, both predicted and with good wavelengths, because three times as many configurations are included and because there are now much better laboratory data. The energy levels are from the NIST website [9] and from more recent literature. The total number of lines stands at 544 million of which 2.11 million have good wavelengths. I expect that the total number of lines will double. Progress, of course, depends on access to funding. When computations with the necessary information are available from others, I am happy to use those data instead of repeating the work.

As the new calculations accumulate I put the results into the /atoms directory on my website, kurucz.harvard.edu. These include the input and output files of the least-squares fits to the energy levels, energy level tables, with energy, J, identification, strongest eigenvector components, lifetime, A-sum, C_4, C_6, and Landé g. The sums are complete up to the first (n = 10) energy level not included. There are electric dipole (E1), magnetic dipole (M1), and electric quadrupole (E2) line lists. Radiative, Stark, and van der Waals damping constants and Landé g values are automatically produced for each line. Branching fractions are also computed. Hyperfine and isotopic splittings are included when the data exist but not automatically. Eigenvalues are replaced by measured energies so that lines connecting measured levels have the correct wavelengths. Most of the lines have uncertain wave-

lengths because they connect predicted rather than measured levels. Measured or estimated widths of autoionizing levels will be included when available. The partition function is tabulated for a range of densities.

For many of the ions, tables of laboratory data are included with *gf* values taken from the NIST website and from more recent literature. In these cases two versions of each line list are given, one with my semiempirical calculations and the other in which my lines are replaced by the laboratory data where they exist.

Generally, low configurations that have been well studied in the laboratory produce good lifetimes and *gf* values, while higher configurations that are poorly observed and are strongly mixed are not well constrained in the least squares fit and necessarily produce poorer results and large scatter. My hope is that the predicted energy levels can help laboratory spectroscopists to identify more levels and further constrain the least squares fits. From my side, I check the computed *gf* values in spectrum calculations by comparing to observed spectra. I adjust the *gf* values so that the spectra match. Then I search for patterns in the adjustments that suggest corrections in the least squares fits.

4. Line lists

The directories /linelists/gfnew and /linelists/gfpred have the merged line lists from /atoms.

All the lines with good wavelengths listed in Table 1 plus data for other ions in the old collection /linelists/gfall that have been taken from the literature (not necessarily up to date) have been merged into files sorted by air wavelength, gfall.dat; vacuum wavelength, gfallvac.dat; and wavenumber, gfallwn.dat. These files include the laboratory *gf* values where available. These files may be updated frequently when I compute new ions or fix errors. If the file /atoms/completed.txt has more recent ion dates than the date of gfall.dat, there are new ions in /atoms waiting to be added.

All the lines with predicted wavelengths listed in Table 1 have been merged into an 88 GB file, sorted by air wavelength, and then compressed into file gfall.predall-gz in directory /linelists/gfpred. The uncompressed file can be used directly to compute spectra in the same way as gfall.dat. Both files must be used to include all the lines. Other packed formats with vacuum wavelengths will be available where all the data necessary for computing spectra or opacities have been reduced to 48 ascii bytes per line. There will also be a binary version with 16 bytes per line that can be fitted into memory.

5. Molecules

I am concentrating on atomic lines first, but since molecules are present in the spectra, they have to be included just to verify the atomic data.

I produced most of my molecular line lists in the 1970s and 1980s. Since then there have been many FTS measurements that have yielded better line positions, better energy levels, and better constants. Line lists are available on a number of websites. The ExoMol website run by Tennyson's group at University College London has many molecular line lists and is being filled with more. There are still gaps in band coverage and isotopologues in the new work. I have updated my line lists using the new data in combination with my old. When I get time I will update all my diatomics and add additional molecules including ions that are missing from my line lists. I will also try to add triatomics so I can work on carbon stars.

My old line lists for C_2, CO, H_2, MgH, NH, and SiO are in directory /molecules/old.

Line lists found on the web for AlO, C_2, CaH, CaO, CN, CO, CrH, FeH, H_2, H_2O, H_3^+, NaH, OH, SiH, TiO, and VO are in directory /molecules. These have all been put into my format. References are given in .readme files.

Most of these molecular line lists have been merged into file diatomics.asc in directory /molecules/oldandnew.

6. Spectrum analysis using stellar atlases as the laboratory source

Chemically peculiar, or CP, stars are early type stars with large over- and underabundances. They can have very small projected rotation velocities, hence narrow lines. Using my calculations Fiorella Castelli has determined 126 new 4d, 5d, 6d, and 4f levels of Fe II in HR6000 [10], which added more than 18 000 lines. She has also determined 73 new Mn II levels from spectra of HD175460 [11]. It would make sense to use a large amount of telescope time to make high-resolution, high-signal-to-noise atlases in the UV, visible, and infrared of selected CP stars so that as many elements as possible can be analyzed to higher energies than are feasible in the lab.

Ruth Peterson looks for unidentified features in Space Telescope UV spectra over a range of low-abundance stars with various effective temperatures and gravities. With low abundances, blending is reduced. She determines the ionization and Boltzmann behavior and then looks for lines in my predicted line list and shifts them in wavenumber to determine the energy level that may produce a match to the observed. If three or more other significant lines from that same energy level match throughout the whole spectrum, that level is assumed to be real. I then recompute the line list using the new energy levels to get improved predictions.

Peterson and Kurucz [12] listed 65 new Fe I levels that produced thousands of new lines. Peterson, Kurucz, and Ayres[2] have identified 59 additional Fe I levels and lines from recently obtained Space Telescope spectra. That work is continuing through support from the Space Telescope Science Institute.

7. Conclusion

Inclusion of heavier elements, higher stages of ionization, additional molecules, and higher energy levels will increase the opacity in stellar atmosphere, pulsation, stellar interior, asteroseismology, nova, supernova, and other radiation hydrodynamics calculations. Detailed and more complete line lists will allow more accurate interpretation of features in spectra and the more accurate determination of stellar properties at any level from elementary 1D approximations to the most sophisticated 3D time-dependent treatments.

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