Including All the Lines: Data Releases for Spectra and Opacities through 2017

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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 850 million lines for elements up through Zn and for the 4d elements from Sr through Pd. Of these, 2.31 million lines are between known energy levels so have good wavelengths for computing spectra. Work is continuing on Ga to Rb and on heavier elements. Data for each ion and merged line lists are available on my website kurucz.harvard.edu.

1. Introduction

I described the “Including All the Lines" project at ASOS10 in Berkeley in 2010 (Kurucz 2011). 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. In 2016 I gave a progress report at the ASOS12 meeting in São Paulo (Kurucz 2017). Here I report on the current status through 2017. Refer to the earlier papers for a discussion of the history, the motivation for the "Including All the Lines" project, molecular line lists, and using stellar spectra as the laboratory source for finding high energy levels. See also /papers/kalamazoo/progress2017.pdf on my website.

2. 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 9 or 10 ions for Ca through Zn. Most of the first five ions of the 4d group Sr through Cd have been completed. I have much work still ahead: Ga-Y, In-Ba, lanthanides, heavy elements, and higher ions for the 3d group.

All of the previous work by Kurucz & Peytremann (1975) and by Kurucz (1988) has been replaced. There are an order of magnitude more lines, both predicted and with good wavelengths, because 3 times as many configurations are included and because there are now much better laboratory data. The energy levels are from the NIST web site (Kramida et al. 2015) and from more recent literature. The total number of lines stands at 850 million of which 2.13 million have good wavelengths. I expect that the total number of lines will be more than one billion. 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 web site, 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, 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 splitting are included when the data exist but not automatically. Eigenvalues are replaced by measured energies so that lines connecting measured levels have correct wavelengths. Most of the lines have uncertain wavelengths 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 web site 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 the 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.

3. 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 a 138GB 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.

4. 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.

References

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Table 1. Partial list of ions completed thus far

	config.		levels		E1 lines		
	even	odd	even	odd	total	good wl	date
Li I	35	32	59	59	938	938	9feb15
F I	48	46	997	962	131375	5461	17jan15
F II	59	60	2026	2214	206549	9355	11jan15
F III	64	60	2033	1851	389119	9835	29dec14
F IV	61	61	1500	1480	342404	4413	18oct16
F V	58	54	807	762	93392	3208	15oct16
F VI	61	58	366	320	42842	3788	21oct16
Ar I	52	53	405	396	49824	16649	2sep11
Ar II	47	47	1001	1024	230953	17188	2sep11
Ar III	48	48	1682	1790	419776	1881	2sep11
Ar IV	33	34	1278	1111	409425	486	2aug16
Ar V	61	61	1616	1638	446472	325	29jul16
Ar VI	61	61	668	751	137526	327	5aug16
Cr I	47	40	18842	18660	2751796	37147	22jan16
Cr II	61	61	13767	15890	8683460	90613	27jan16
Cr III	61	61	6560	7526	6436134	13150	22jul14
Cr IV	61	61	2094	2318	1044865	2590	6sep15
Cr V	61	61	509	636	109427	252	5sep15
Cr VI	33	32	134	147	10125	357	17aug15
Cr VII	32	33	245	253	121069	590	13aug15
Cr VIII	56	52	1555	1281	729126	35	2apr16
Cr IX	53	54	1453	1456	756558	80	9apr16
Zn I	72	72	566	681	34135	6282	4jan12
Zn II	61	61	926	1286	31563	968	13jan12
Zn III	61	61	4303	5758	640536	12674	13jan12
Zn IV	61	61	10252	11429	5715894	7214	12jun16
Zn V	60	50	18353	19364	13806567	2544	16jun16
Zn VI	44	39	18343	19517	21467731	1614	3jun16
Zn VII	46	41	18208	19238	24491877	1498	24jun16
Zn VIII	61	61	13706	15660	21677814	3	13jul16
Zn IX	61	61	6560	7526	7226420	0	14jul16
Ru I	60	50	17803	18850	7627968	8368	7aug17
Ru II	44	39	18669	19652	15380475	5410	10jul17
Ru III	53	48	18322	19924	23085495	78	1sep17
Ru IV	61	61	13706	15890	33857562	0	4sep17
Ru V	61	61	6560	7550	10821990	0	5sep17