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 to Zn and for the 4d elements from Sr through Pd. Of these, 2.31 million lines are between known energy levels, so they 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 the ASOS10 meeting in Berkeley, CA, in August 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 July 2016 I gave a progress report at the ASOS12 meeting in São Paulo, Brazil (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. The full 2017 progress report[1] can also be obtained online from my website[2].

2. Progress Report

Tables 1–5 show 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.

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[1] http://kurucz.harvard.edu/papers/kalamazoo/progress2017.pdf

[2] http://kurucz.harvard.edu

The whole table[3] can be accessed online. 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, the lanthanides, heavy elements, and higher ions for the 3d group.

All the previous work by Kurucz & Peytremann (1975) and Kurucz (1988) 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 (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 website. 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 factor. 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 such 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 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 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

[3] `http://kurucz.harvard.edu/atoms/completed.txt`

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 138 GB file, sorted by air wavelength, and then compressed into file *gfall.predall-gz* in the 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

Kramida, A., Ralchenko, Yu., Reader, J., & the NIST ASD Team, 2015, NIST Atomic Spectra Database (ver. 5.3 and earlier versions), `http://physics.nist.gov/asd`

Kurucz, R. L. 1988, in Proceedings of the 20th General Assembly, edited by M. McNally (Dordrecht, The Netherlands: Kluwer Academic Publishers), vol. XXB of Trans. IAU, 168

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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
Be I	61	58	366	320	23574	3822	2mar15
Be II	35	32	59	64	1418	714	6may15
B I	64	65	744	805	22012	1370	15may15
B II	61	61	366	404	34046	5130	24apr15
B III	35	32	59	64	1436	794	25apr15
C I	72	74	1722	1778	250828	33037	19jun15
C II	58	54	807	762	26735	4148	3jan14
C III	61	61	366	404	38826	8173	4nov13
C IV	67	62	358	44	9408	2028	20sep14
N I	77	72	2322	2155	356876	14484	4aug14
N II	60	60	1566	1578	169232	4105	19jul14
N III	80	77	972	1005	83172	12770	32jul14
N IV	63	58	374	320	39056	11171	29may15
N V	67	62	358	443	9969	1337	17may15
O I	61	61	2074	1848	109396	13484	16dec13
O II	60	60	1886	1851	296883	9598	26apr14
O III	61	61	1500	1480	268985	8665	30may14
O IV	58	54	807	762	58706	5742	3mar11
O V	61	58	366	320	41072	3453	23may15
O VI	67	62	358	443	9508	1243	19may15
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	42824	3788	21oct16
Ne I	54	55	397	380	49187	15361	12may13
Ne II	48	46	997	962	178364	18465	30jan15
Ne III	59	60	2026	2214	307791	9464	21jan15
Ne IV	64	60	2033	1851	479643	7654	2oct16
Ne V	61	61	1500	1480	405039	3700	6oct16
Ne VI	58	54	807	762	107912	3292	13oct16
Na I	68	79	1255	1894	32848	4456	11sep12
Na II	54	55	397	380	52696	4161	13may13
Na III	48	46	997	962	211479	1867	14jun13
Na IV	59	60	2826	2214	506803	1372	29aug16
Na V	64	60	2033	1851	563935	1475	3oct16
Na VI	61	61	1500	1480	507933	2146	10oct16
Mg I	61	61	272	316	22612	11127	14jul09
Mg II	44	43	155	169	6018	2832	1feb13
Mg III	34	35	257	260	21805	1839	13dec12
Mg IV	48	46	997	962	242202	3246	16sep16
Mg V	59	60	2826	2214	692686	750	24aug16
Mg VI	64	60	2033	1851	656167	2073	20sep16

Table 2. Partial list of ions completed thus far

	config.		levels		E1 lines		
	even	odd	even	odd	total	good wl	date
Al I	67	71	936	952	29081	3255	8may12
Al II	66	58	435	504	31420	4847	21may12
Al III	44	43	155	124	5145	2839	11feb13
Al IV	40	41	309	308	29977	1745	16aug16
Al V	46	48	997	962	273987	2826	13sep16
Al VI	59	60	2826	2214	852042	1003	28aug16
Si I	61	61	1616	1588	190165	10578	16jun12
Si II	61	65	892	872	36508	3006	5jun15
Si III	54	50	363	424	25109	2726	9mar13
Si IV	44	42	155	124	5033	2440	12feb13
Si V	34	35	257	260	22442	1156	17aug16
Si VI	48	46	997	962	279058	1868	9sep16
P I	32	34	1278	1109	202300	12272	22mar13
P II	61	61	1616	1638	217038	2954	6feb12
P III	61	61	668	751	60141	2223	24mar13
P IV	60	56	435	496	43431	4807	14aug16
P V	44	42	155	124	4941	587	18aug16
P VI	34	35	257	260	27643	487	18aug16
S I	61	61	2161	2270	225605	24722	21oct04
S II	34	32	1278	1109	275137	7275	28mar13
S III	61	61	1616	1638	298390	433	27apr13
S IV	61	61	668	751	87349	2968	7aug16
S V	54	50	363	424	34300	2182	8aug16
S VI	44	42	155	124	4985	782	19aug16
Cl I	61	61	865	863	256337	17528	4mar13
Cl II	61	61	1604	1506	258102	9561	25feb13
Cl III	34	33	1278	1111	364878	949	3mar13
Cl IV	61	61	1616	1638	369835	238	31jul16
Cl V	61	61	668	751	108825	153	5aug16
Cl VI	61	61	467	540	69047	610	8aug16
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
K I	83	88	1497	1388	49987	2472	5feb12
K II	52	53	405	396	55355	1125	18mar12
K III	47	47	1001	1024	313550	211	21feb13
K IV	53	54	1555	1201	548287	109	3aug16
K V	33	34	1278	1111	447194	146	31jul16
K VI	61	61	1616	1638	508408	75	28jul16

Table 3. Partial list of ions completed thus far

	config.		levels		E1 lines		
	even	odd	even	odd	total	good wl	date
Ca I	61	61	515	612	46062	25251	2jun13
Ca II	57	56	1497	1388	50436	2433	13nov10
Ca III	52	53	405	396	58089	2897	26jan12
Ca IV	56	52	1555	1201	569544	1693	11apr16
Ca V	53	54	1453	1456	621461	121	10apr16
Ca VI	34	33	1278	1111	492358	111	13apr16
Ca VII	67	65	1802	1742	601122	386	18apr16
Ca VIII	61	61	668	751	172048	462	21apr16
Ca IX	68	80	595	832	80906	1042	25apr16
Sc I	61	61	2014	2318	737992	15546	17feb09
Sc II	61	61	509	644	116491	3436	9jan09
Sc III	39	38	134	147	5271	1313	16feb13
Sc IV	32	33	245	252	22348	1599	5jul15
Sc V	56	52	1555	1201	645368	2180	20oct09
Sc VI	53	54	1454	1456	671701	119	9apr16
Sc VII	34	33	1278	1111	532198	124	14apr16
Sc VIII	67	65	1802	1742	669845	72	19apr16
Sc IX	61	61	668	751	190211	387	27apr16
Ti I	61	61	6628	7350	5074395	35085	5feb16
Ti II	61	61	2096	2318	897985	8249	12feb16
Ti III	73	68	3636	3845	499739	4090	27aug10
Ti IV	39	38	134	147	7764	1844	19feb13
Ti V	32	33	245	252	116840	498	19jul15
Ti VI	56	52	1555	1201	695487	2844	25mar16
Ti VII	53	54	1454	1456	702567	143	8apr16
Ti VIII	34	33	1278	1111	551270	128	14apr16
Ti IX	67	65	1802	1742	719452	79	20apr16
V I	61	61	13767	15952	7043556	23342	11aug11
V II	61	61	6740	7422	4347535	18752	9jul13
V III	61	61	2094	2318	966528	9892	15sep10
V IV	61	61	509	636	108495	1304	15aug15
V V	33	32	134	147	9634	450	16aug15
V VI	32	33	245	252	119797	526	7aug15
V VII	56	52	1555	1201	720329	36	1apr16
V VIII	53	54	1454	1456	737661	92	9apr16
V IX	34	33	2378	1111	576296	111	15apr16
Cr I	47	40	18842	18660	2751796	37147	22jan16
Cr II	61	61	13767	15890	8683460	90613	27jan16
Cr III	61	61	6508	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

Table 4. Partial list of ions completed thus far

	config.		levels		E1 lines		
	even	odd	even	odd	total	good wl	date
Mn I	44	39	18343	19652	1481464	16798	21jan07
Mn II	50	41	19686	19870	5136978	42000	2sep16
Mn III	51	61	13706	15890	10525088	17294	23jul10
Mn IV	61	61	6560	7526	6731193	2742	19aug15
Mn V	61	61	2094	2461	1140407	917	8sep15
Mn VI	61	61	747	820	222649	1468	14sep15
Mn VII	33	32	134	147	10236	204	18aug15
Mn VIII	32	33	245	253	121463	126	14aug15
Mn IX	56	52	1555	1281	738190	39	6apr16
Fe I	61	50	18655	18850	7500416	126288	2feb17
Fe II	46	39	19771	19652	7834553	124654	8dec13
Fe III	49	41	19720	19820	10799751	37093	25jun15
Fe IV	61	54	13767	14211	14617228	8408	24aug06
Fe V	61	61	6560	7526	7785320	11417	21aug06
Fe VI	73	73	2094	2496	9072714	3534	16aug10
Fe VII	85	86	7132	7032	2816992	2326	9jul10
Fe VIII	52	52	1365	1244	220166	233	20jul10
Fe IX	32	33	245	252	123563	281	11aug15
Fe X	56	52	1555	1281	749848	346	6apr16
Co I	61	61	10920	13085	3771900	15441	24oct08
Co II	61	50	18655	19364	10050728	23355	16nov06
Co III	44	39	18343	19652	11515139	9356	23aug10
Co IV	49	41	19720	19820	14416296	9178	23aug15
Co V	61	61	13767	15693	17989106	7875	24aug15
Co VI	61	61	6560	7526	7226567	3725	3sep15
Co VII	73	74	12727	9458	11278682	1153	16mar16
Co VIII	61	61	509	820	156222	801	21feb16
Co IX	52	52	1365	1244	155055	180	18mar16
Ni I	61	61	4303	5758	732160	9663	29oct08
Ni II	61	61	10270	11429	3645991	55590	23oct10
Ni III	61	50	18655	19364	11120833	21251	3feb07
Ni IV	44	39	18343	19517	17912731	5659	1jun16
Ni V	46	41	10637	19238	15622452	10637	23nov09
Ni VI	61	61	13706	15792	21466118	12219	27jun16
Ni VII	73	73	24756	19567	28328012	3502	25jun10
Ni VIII	73	73	12714	8903	12308126	758	23jun10
Ni IX	85	86	7132	7032	2671345	253	24jun10
Ni X	52	52	1365	1208	285029	235	2jul10
Cu I	61	61	920	1260	28112	5720	11jun12
Cu II	61	61	4303	5758	622985	14959	28sep11
Cu III	61	61	10270	11429	5258607	17539	15mar13
Cu IV	61	50	19364	17365	15717162	9559	25sep15
Cu V	44	39	18343	19517	19912950	6164	27may16
Cu VI	46	41	18208	19238	28428043	4268	19jun16
Cu VII	61	61	13706	15660	20890885	2406	28jun16
Cu VIII	61	61	6560	7526	7176844	0	15jun16
Cu IX	61	61	2094	2560	1245825	0	16jul16
Cu X	85	86	508	3002	2910966	159	28may10

Table 5. Partial list of ions completed thus far

	config.		levels		E1 lines		
	even	odd	even	odd	total	good wl	date
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
Sr I	61	61	519	628	42301	22686	9jul12
Sr II	36	36	141	155	5993	670	24jan17
Y I	61	61	1634	2141	59226	5393	12dec06
Y II	69	65	806	930	145597	7213	30sep11
Zr I	61	61	6560	7550	5064270	6200	20jun17
Zr II	61	61	1880	2141	1026414	1880	18jun17
Zr III	62	61	515	652	117743	2360	25jun17
Nb I	61	61	13706	15890	7264287	10760	18may17
Nb II	61	61	6560	7550	8320614	15048	28may17
Nb III	61	61	1880	2141	1050775	4009	24sep17
Mo I	53	48	18322	19924	3829733	13848	15apr17
Mo II	61	61	13706	15890	19869870	13272	4may17
Mo III	61	61	6560	7550	9947505	12387	19sep17
Mo IV	61	61	1880	2141	1058760	2804	23sep17
Tc I	44	39	18669	19652	5096138	8815	7oct17
Tc II	53	48	18322	19924	11149162	119	29sep17
Tc III	61	61	13786	15890	32046068	0	26sep17
Tc IV	61	61	6560	7570	10012365	0	21sep17
Tc V	61	61	1880	2141	1057551	0	25sep17
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	70	1sep17
Ru IV	61	61	13706	15890	33857562	0	4sep17
Ru V	61	61	6560	7550	10821990	0	5sep17
Rh I	61	61	10386	13679	3043408	2332	19aug17
Rh II	60	50	17803	18850	13817566	1527	20aug17
Rh III	44	39	18669	19652	28483809	3969	6sep17
Rh IV	61	61	18322	19924	23058802	0	5sep17
Rh V	61	61	13766	15890	37530563	0	6sep17
Pd I	61	61	4295	5934	571621	2996	6sep17
Pd II	61	61	10346	13679	5191374	4558	22sep17
Ba I	61	61	519	628	66443	5933	23mar17
Ba II	34	30	59	60	1422	703	23mar17