

Including All the Lines

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Abstract. I present a progress report on including all the lines in the linelists, including all the lines in the opacities, including all the lines in the model atmosphere and spectrum synthesis calculations, producing high-resolution, high-signal-to-noise atlases that show (not quite) all the lines, so that finally we can determine the properties of stars from a few of the lines.

Keywords: atomic data — molecular data — atlases — sun: atmosphere — sun: abundances
— stars: atmospheres — stars: abundances — supernovae: general

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INTRODUCTION

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 calculation of the first 9 ions of the iron group elements shown in Table 1 using my versions of Cowan's atomic structure programs (Kurucz 1988) [1]. 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 linelists for diatomic molecules including 15 million lines of H₂, CH, NH, OH, MgH, SiH, C₂, CN, CO, SiO, and TiO for a total of 58 million lines.

I then tabulated 2 nm resolution opacity distribution functions from the line list for temperatures from 2000 to 200000K and for a range of pressure suitable for stellar atmospheres (Kurucz 1992) [2].

Using the ODFs I computed a theoretical solar model (Kurucz 1992) [3] with the solar effective temperature and gravity, the current solar abundances from Anders and

Table 1. Iron group lines computed at San Diego Supercomputer Center 1988

	I	II	III	IV	V	VI	VII	VIII	IX
Ca	48573	4227	11740	113121	330004	217929	125560	30156	22803
Sc	191253	49811	1578	16985	130563	456400	227121	136916	30587
Ti	867399	264867	23742	5079	37610	155919	356808	230705	139356
V	1156790	925330	284003	61630	8427	39525	160652	443343	231753
Cr	434773	1304043	990951	366851	73222	10886	39668	164228	454312
Mn	327741	878996	1589314	1033926	450293	79068	14024	39770	147442
Fe	789176	1264969	1604934	1776984	1008385	475750	90250	14561	39346
Co	546130	1048188	2198940	1569347	2032402	1089039	562192	88976	15185
Ni	149926	404556	1309729	1918070	1971819	2211919	967466	602486	79627

Grevesse (1989) [4], mixing length to scale height ratio $l/H = 1.25$, and constant microturbulent velocity 1.5 km/s. It generally matched the observed energy distribution from Neckel and Labs (1984) [5].

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.

PROBLEMS

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

Since 1965 the Fe abundance 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 km/s. My 1D models still have mixing-length convection, but now with a depth-dependent microturbulent velocity that scales with the convective velocity. 3D 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 linelists. Table 2 is an outline for the Fe II line calculation then. The higher energy levels that produce series of lines that merge into ultraviolet continua were not included. Those levels also produce huge numbers of weaker lines in the visible and infrared 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.

Table 2. Fe II in 1988

Based on Johansson (1978) [6]

Even: 22 configurations; 5723 levels; 354 known levels;

729 Hamiltonian parameters, all CI; 46 free LS parameters; dev 142 cm⁻¹

		d ⁷			
d ⁶ 4s	d ⁵ 4s ²	d ⁶ 4d	d ⁵ 4s4d	d ⁴ 4s ² 4d	d ⁵ 4p ²
d ⁶ 5s	d ⁵ 4s5s	d ⁶ 5d	d ⁵ 4s5d	d ⁶ 5g	
d ⁶ 6s	d ⁵ 4s6s	d ⁶ 6d	d ⁵ 4s6d	d ⁶ 6g	
d ⁶ 7s		d ⁶ 7d		d ⁶ 7g	
d ⁶ 8s		d ⁶ 8d			
d ⁶ 9s					

Odd: 16 configurations; 5198 levels; 435 known levels;

541 Hamiltonian parameters, all CI; 43 free LS parameters; dev 135 cm⁻¹

d ⁶ 4p	d ⁵ 4s4p	d ⁶ 4f	d ⁵ 4s4f	d ⁴ 4s ² 4p
d ⁶ 5p	d ⁵ 4s5p	d ⁶ 5f		
d ⁶ 6p	d ⁵ 4s6p	d ⁶ 6f		
d ⁶ 7p	d ⁵ 4s7p			
d ⁶ 8p	d ⁵ 4s8p			
d ⁶ 9p				

Total E1 lines saved 1264969

E1 lines with good wavelengths 45815

EXAMPLES OF NEW CALCULATIONS

Here I show sample statistics from my new semiempirical calculations for Fe II, Ni I, and Co I to illustrate how important it is to do the basic physics well and how much data there are to deal with. Ni, Co, and Fe are prominent in supernovas, including both radioactive and stable isotopes. There is not space here for the lifetime and gf comparisons. 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.

As the new calculations accumulate I will put on my web site the output files of

the least-squares fits to the energy levels, energy level tables, with E, 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 will be electric dipole, magnetic dipole, and electric quadrupole 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 will be 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. Laboratory measurements of gf values and lifetimes will be included. Measured or estimated widths of autoionizing levels will be included when available. The partition function will be tabulated for a range of densities.

When computations with the necessary information are available from other workers, I am happy to use those data instead of repeating the work.

Once the linelist for an ion or molecule is validated it will be incorporated into the wavelength sorted linelists on my website for computing opacities or detailed spectra. The web directories are kurucz.harvard.edu/atoms and [/molecules](http://kurucz.harvard.edu/molecules) for the details and [/linelists](http://kurucz.harvard.edu/linelists) for the completed linelists.

Table 3 presents line statistics from some of my recent calculations that show an order of magnitude increase over my earlier work. Table 4 shows my estimate that my linelists will have several billion atomic and molecular lines if I can continue my work.

Fe II

Based on Johansson (1978) [6] and on more recent published and unpublished data. Johansson had data for more than 100 energy levels that I do not yet have.

Even: 46 configurations; 19771 levels; 403 known levels;

2645 Hamiltonian parameters, all CI; 58 free LS parameters; dev 56 cm⁻¹

d ⁷								
d ⁶ 4s	d ⁵ 4s ²	d ⁶ 4d	d ⁵ 4s4d			d ⁴ 4s ² 4d	d ⁵ 4p ²	
d ⁶ 5s	d ⁵ 4s5s	d ⁶ 5d	d ⁵ 4s5d	d ⁶ 5g	d ⁵ 4s5g	d ⁴ 4s ² 5s		
d ⁶ 6s	d ⁵ 4s6s	d ⁶ 6d	d ⁵ 4s6d	d ⁶ 6g	d ⁵ 4s6g			
d ⁶ 7s	d ⁵ 4s7s	d ⁶ 7d	d ⁵ 4s7d	d ⁶ 7g	d ⁵ 4s7g	d ⁶ 7i	d ⁵ 4s7i	
d ⁶ 8s	d ⁵ 4s8s	d ⁶ 8d	d ⁵ 4s8d	d ⁶ 8g	d ⁵ 4s8g	d ⁶ 8i	d ⁵ 4s8i	d ⁵ 4s9i
d ⁶ 9s	d ⁵ 4s9s	d ⁶ 9d	d ⁵ 4s9d	d ⁶ 9g	d ⁵ 4s9g	d ⁶ 9i	d ⁵ 4s9i	d ⁶ 9l

Odd: 39 configurations; 19652 levels; 492 known levels;

2996 Hamiltonian parameters, all CI; 51 free LS parameters; dev 75 cm⁻¹

d ⁶ 4p	d ⁵ 4s4p	d ⁶ 4f	d ⁵ 4s4f			d ⁴ 4s ² 4p	d ⁴ 4s ² 4f
d ⁶ 5p	d ⁵ 4s5p	d ⁶ 5f	d ⁵ 4s5f			d ⁴ 4s ² 5p	
d ⁶ 6p	d ⁵ 4s6p	d ⁶ 6f	d ⁵ 4s6f	d ⁶ 6h	d ⁵ 4s6h		
d ⁶ 7p	d ⁵ 4s7p	d ⁶ 7f	d ⁵ 4s7f	d ⁶ 7h	d ⁵ 4s7h		
d ⁶ 8p	d ⁵ 4s8p	d ⁶ 8f	d ⁵ 4s8f	d ⁶ 8h	d ⁵ 4s8h	d ⁶ 8k	d ⁵ 4s8k
d ⁶ 9p	d ⁵ 4s9p	d ⁶ 9f	d ⁵ 4s9f	d ⁶ 9h	d ⁵ 4s9h	d ⁶ 9k	d ⁵ 4s9k

Total E1 lines saved new / old = 7719063 / 1254969 ratio = 6
E1 lines with good wavelengths new / old = 81225 / 45815 ratio = 1.8

Forbidden lines	even	odd
total M1 lines saved	1852641	2468074
with good wavelengths	28102	41374
between metastable	1180	0

total E2 lines saved	10347332	13179033
with good wavelengths	49019	71225
between metastable	1704	0

isotopic components	⁵⁴ Fe	⁵⁶ Fe	⁵⁷ Fe	⁵⁸ Fe
fractional abundances	.059	.9172	.021	.0028

⁵⁷Fe has not yet been measured because it has hyperfine splitting. Rosberg, Litzén, and Johansson (1993) [7] have measured ⁵⁶Fe–⁵⁴Fe in 9 lines and ⁵⁸Fe–⁵⁶Fe in one line. I split the computed lines by hand.

Ni I

Ni I mostly based on Litzén, Brault, and Thorne (1993) [8] with **isotopic splitting**.

Total E1 lines saved new / old = 732160 / 149926 ratio = 4.9
E1 lines with good wavelengths new / old = 9663 / 3949 ratio = 2.4

isotope	⁵⁶ Ni	⁵⁷ Ni	⁵⁸ Ni	⁵⁹ Ni	⁶⁰ Ni	⁶¹ Ni	⁶² Ni	⁶³ Ni	⁶⁴ Ni
fraction	.0	.0	.6827	.0	.2790	.0113	.0359	.0	.0091

There are 5 stable isotopes. There are measured splittings for 326 lines from which I determined 131 energy levels relative to the ground. These levels are connected by **11670 isotopic lines**. Hyperfine splitting was included for ⁶¹Ni but only 6 levels have been measured which produce 4 lines with 38 components. A pure isotope laboratory analysis is needed. Ni I lines are asymmetric from the splitting and they now agree in shape with lines in the solar spectrum.

Co I

Co I based on Pickering and Thorne (1996) [9] and on Pickering (1996) [10] with hyperfine splitting.

Total E1 lines saved new / old = 3771908 / 546130 ratio = 6.9
 E1 lines with good wavelengths new / old = 15441 / 9879 ratio = 2.4

⁵⁹Co is the only stable isotope. Hyperfine constants have been measured in 297 levels which produce **244264 component E1 lines**. I have not yet computed the M1 or E2 components. The new calculation greatly improves the appearance of the Co I lines in the solar spectrum.

Table 3. Sample recent calculations

		config		levels		good wl	E1 lines	
		even	odd	even	odd		total	old
Fe	I	61	50	18655	18850	93508	6029023	789176
Fe	II	46	39	19771	19652	85362	7615097	1264969
Fe	III	49	41	19720	19820	33982	9770250	1604934
Fe	IV	61	54	13767	14211	8408	14617228	1776984
Fe	V	61	61	6560	7526	11417	7785320	1008385
Fe	VI	61	61	2094	2496	3535	1386203	475750
S	I	61	61	2161	2270	24722	225605	
Sc	I	61	61	2014	2318	15546	737992	191253
Sc	II	61	61	509	644	3436	116491	49811
Ti	I	61	61	6628	7350	33625	4754432	867399
Mn	I	44	39	18343	19652	16798	1481464	327741
Co	I	61	61	10920	13085	15441	3771900	546130
Co	II	61	50	18655	19364	23355	10050728	1361114
Ni	I	61	61	4303	5758	9663	732160	149925
Ni	II	61	61	10270	11429	55590	3645991	404556
Ni	III	61	50	18655	19364	21251	11120833	1309729
Cu	I	61	61	920	1260	5720	28112	
Cu	II	61	61	4303	5758	14959	622985	
Cu	IV	55	50	9563	17365	9563	11857712	
Y	I	61	61	1634	2141	5393	59226	

Total: new / old = 100 million / 12 million ratio = 8

Table 4. Estimated lines in 3d and 4d group sequences (in millions)

	I	II	III	IV	V	VI	VII	VIII	IX	X	...
Ca	.05										
Sc	.7	.05									
Ti	5	.7	.05								
V	14	5	.7	.05							
Cr	10	14	5	.7	.05						
Mn	1.5	10	14	5	.7	.05					
Fe	6	7	10	14	5	.7	.05				
Co	4	10	7	10	14	5	.7	.05			
Ni	.7	4	10	7	10	14	5	.7	.05		
Cu	.03	.6	4	10	7	10	14	5	.7	.05	
Zn	.1	.03	.6	4	10	7	10	14	5	.7	...
Ga		.1	.03	.6	4	10	7	10	14	5	...
Ge			.1	.03	.6	4	10	7	10	14	...
As				.1	.03	.6	4	10	7	10	...
Se					.1	.03	.6	4	10	7	...
Br						.1	.03	.6	4	10	...
Kr							.1	.03	.6	4	...
Rb								.1	.03	.6	...
Sr	.05								.1	.03	...
Y	.7	.05								.1	...
Zr	5	.7	.05								
Nb	14	5	.7	.05							
Mo	10	14	5	.7	.05						
[Tc]	1.5	10	14	5	.7	.05					
Ru	6	7	10	14	5	.7	.05				
Rh	4	10	7	10	14	5	.7	.05			
Pd	.7	4	10	7	10	14	5	.7	.05		
Ag	.03	.6	4	10	7	10	14	5	.7	.05	
Cd	.1	.03	.6	4	10	7	10	14	5	.7	...
In		.1	.03	.6	4	10	7	10	14	5	...
Sn			.1	.03	.6	4	10	7	10	14	...
Sb				.1	.03	.6	4	10	7	10	...
Te					.1	.03	.6	4	10	7	...
I						.1	.03	.6	4	10	...
Xe							.1	.03	.6	4	...
Cs								.1	.03	.6	...
Ba									.1	.03	...

TOTAL 3d > 500 MILLION

TOTAL 4d > 500 MILLION

+ LANTHANIDE SEQUENCES > 1000 MILLION

+ ALL THE OTHER ELEMENT SEQUENCES

TiO and H₂O

These are examples of incorporating data from other researchers.

Schwenke (1998) [11] calculated energy levels for TiO including in the Hamiltonian the 20 lowest vibration states of the 13 lowest electronic states of TiO (singlets a, b, c, d, f, g, h and triplets X, A, B, C, D, E) and their interactions. He determined parameters by fitting the observed energies or by computing theoretical values. Using Langhoff's transition moments [12] Schwenke generated a linelist for J = 0 to 300 for the

isotopomers $^{46}\text{Ti}^{16}\text{O}$ $^{47}\text{Ti}^{16}\text{O}$ $^{48}\text{Ti}^{16}\text{O}$ $^{49}\text{Ti}^{16}\text{O}$ $^{50}\text{Ti}^{16}\text{O}$

fractional abundances .080 .073 .738 .055 .054

My version has 37,744,499 lines.

Good analyses and a similar semiempirical treatment are needed for CaOH, ScO, VO, YO, ZrO, LaO, etc.

Partridge and Schwenke (1997) [13] treated H₂O semiempirically. They included isotopomers H₂¹⁶O, H₂¹⁷O, H₂¹⁸O, and HD¹⁶O. My version has 65,912,356 lines. I hope to obtain a newer linelist with a billion lines in the near future.

COMPUTING OPACITY

My program DFSYNTH can compute the LTE opacity spectrum of 1 billion lines, at 4 million frequencies, for 1000 T-P pairs, for a range of V_{turb}.

Those spectra can be statistically processed into ODF tables as they are computed, or treated in some other approximation, or they can be saved directly. Instead of dealing with lines, one can just interpolate (and doppler shift) the opacity spectra.

MODEL ATMOSPHERE PROGRAMS

My model atmosphere program ATLAS12 can deal with 1 billion lines by sampling. It preselects into a smaller linelist the lines that are relevant for the model. It defaults to 30000 sampling points but it could sample a million. It can treat arbitrary depth-dependent abundances and velocities.

My program ATLAS9 uses ODFs so it is independent of the number of lines.

ATLASES AND SPECTRUM SYNTHESIS

High-resolution, high-signal-to-noise spectra are needed to test the line data and the spectrum synthesis programs and to determine the stellar parameters.

There are no high quality solar spectra taken above the atmosphere. There are good quality FTS spectra from 2 to 16 microns taken by the ATMOS experiment on the space shuttle.

There are no high or good quality solar spectra in the ultraviolet.

There are various good quality solar spectra taken through the atmosphere. I have been trying to reduce the FTS spectra taken by James Brault from Kitt Peak to produce central intensity, limb intensity, flux, and irradiance atlases.

Color figures for the Kitt Peak Flux Atlas, telluric absorption, the Kitt Peak Irradiance Atlas, irradiance in the H band, and a one-angstrom sample spectrum calculation with the lines labelled are on my website kurucz.harvard.edu/papers/dimitrifest.

CONCLUDING REMARKS

Comments on spectrum synthesis and abundance analysis:

Abundances are generally determined from blended features that must be deconvolved by synthesizing the features including every significant blending line.

In general, one half the discernible lines are missing from the lists of lines with good wavelengths.

Every line has to be adjusted in wavelength, damping constants, and gf value.

Most lines used in abundance analyses are not suitable. Including many lines reduces the accuracy.

We do not know anything with certainty about the sun, except its mass.

Inclusion of heavier elements, higher stages of ionization, additional molecules, and higher energy levels, will increase the opacity in stellar atmospheres, stellar envelopes, stellar interiors, supernovae, galaxies, and the rest of the universe.

Detailed and more complete linelists will allow more accurate interpretation of features in spectra and the determination of stellar properties at any level of radiation hydrodynamics from elementary approximations to the most sophisticated treatments.

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