Including All the Lines

Robert L. Kurucz

Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, U.S.A.

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 H$_2$, CH, NH, OH, MgH, SiH, C$_2$, 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 | 990951 | 366851 | 73222 | 39525 | 164228 | 454312 |
| Cr  | 434773 | 1304043 | 990951 | 366851 | 73222 | 39525 | 164228 | 454312 |
| Mn  | 327741 | 878996 | 1589314 | 1033926 | 450293 | 79068 | 14024 | 39770 | 147442 |
| Fe  | 789176 | 1264969 | 1604934 | 1776984 | 1008385 | 475750 | 90250 | 14565 | 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$^{-1}$

\[
\begin{array}{cccccc}
\text{d}^7 & & & & & \\
\text{d}^6\text{s} & \text{d}^5\text{4}s^2 & \text{d}^6\text{4}d & \text{d}^5\text{4}s\text{4}d & \text{d}^4\text{4}s^2\text{4}d & \text{d}^5\text{4}p^2 \\
\text{d}^6\text{5}s & \text{d}^5\text{4}s\text{5}s & \text{d}^6\text{5}d & \text{d}^5\text{4}s\text{5}d & \text{d}^6\text{5}g \\
\text{d}^6\text{6}s & \text{d}^5\text{4}s\text{6}s & \text{d}^6\text{6}d & \text{d}^5\text{4}s\text{6}d & \text{d}^6\text{6}g \\
\text{d}^6\text{7}s & \text{d}^6\text{7}d & \text{d}^6\text{7}g \\
\text{d}^6\text{8}s & \text{d}^6\text{8}d \\
\text{d}^6\text{9}s \\
\end{array}
\]

Odd: 16 configurations; 5198 levels; 435 known levels;
541 Hamiltonian parameters, all CI; 43 free LS parameters; dev 135 cm$^{-1}$

\[
\begin{array}{cccc}
\text{d}^6\text{4}p & \text{d}^5\text{4}s\text{4}p & \text{d}^6\text{4}f & \text{d}^5\text{4}s\text{4}f & \text{d}^4\text{4}s^2\text{4}p \\
\text{d}^6\text{5}p & \text{d}^5\text{4}s\text{5}p & \text{d}^6\text{5}f \\
\text{d}^6\text{6}p & \text{d}^5\text{4}s\text{6}p & \text{d}^6\text{6}f \\
\text{d}^6\text{7}p & \text{d}^5\text{4}s\text{7}p \\
\text{d}^6\text{8}p & \text{d}^5\text{4}s\text{8}p \\
\text{d}^6\text{9}p \\
\end{array}
\]

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, C₄, C₆, 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 for the details and /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

d⁷
\[d^6s \ d^5s^2 \ d^6d \ d^5s^4d \ d^4s^2d \ d^5p^2 \]
d⁶s \ d⁵s⁵s \ d⁵d \ d⁴s⁵d \ d⁵g \ d⁵s⁵g \ d⁴s⁵s \ d⁴s⁵d

d⁶d \ d⁵s⁶d \ d⁶d \ d⁵s⁶d \ d⁶g \ d⁵s⁶g

d⁶⁷s \ d⁵s⁷s \ d⁶⁷d \ d⁵s⁷d \ d⁶⁷g \ d⁵s⁷g \ d⁶⁷i \ d⁵s⁷i

d⁶⁸s \ d⁵s⁸s \ d⁶⁸d \ d⁵s⁸d \ d⁶⁸g \ d⁵s⁸g \ d⁶⁸i \ d⁵s⁸i \ d⁵s⁹i

d⁷⁹s \ d⁵s⁹s \ d⁶⁹d \ d⁵s⁹d \ d⁶⁹g \ d⁵s⁹g \ d⁶⁹i \ d⁵s⁹i \ d⁶⁹i

Odd: 39 configurations; 19652 levels; 492 known levels;
2996 Hamiltonian parameters, all CI; 51 free LS parameters; dev 75 cm⁻¹
\begin{align*}
d^64p & \quad d^54s4p & \quad d^64f & \quad d^54s4f \\
d^65p & \quad d^54s5p & \quad d^65f & \quad d^54s5f \\
d^66p & \quad d^54s6p & \quad d^66f & \quad d^54s6f \\
d^67p & \quad d^54s7p & \quad d^67f & \quad d^54s7f \\
d^68p & \quad d^54s8p & \quad d^68f & \quad d^54s8f \\
d^69p & \quad d^54s9p & \quad d^69f & \quad d^54s9f \\
\end{align*}

Total E1 lines saved \quad new / old = 7719063 / 1254969 \quad ratio = 6

E1 lines with good wavelengths \quad new / old = 81225 / 45815 \quad ratio = 1.8

Forbidden lines

\begin{align*}
\text{total M1 lines saved} & \quad \text{even} & \quad \text{odd} \\
& \quad 1852641 & \quad 2468074 \\
\text{with good wavelengths} & \quad 28102 & \quad 41374 \\
\text{between metastable} & \quad 1180 & \quad 0 \\
\end{align*}

\begin{align*}
\text{total E2 lines saved} & \quad 10347332 & \quad 13179033 \\
\text{with good wavelengths} & \quad 49019 & \quad 71225 \\
\text{between metastable} & \quad 1704 & \quad 0 \\
\end{align*}

\begin{align*}
isotopic \text{ components} & \quad ^{54}\text{Fe} & \quad ^{56}\text{Fe} & \quad ^{57}\text{Fe} & \quad ^{58}\text{Fe} \\
\text{fractional abundances} & \quad .059 & \quad .9172 & \quad .021 & \quad .0028 \\
\end{align*}

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

\section*{Ni I}

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

\begin{align*}
\text{Total E1 lines saved} & \quad \text{new / old} = 732160 / 149926 \quad \text{ratio} = 4.9 \\
\text{E1 lines with good wavelengths} & \quad \text{new / old} = 9663 / 3949 \quad \text{ratio} = 2.4 \\
isotope & \quad ^{56}\text{Ni} & \quad ^{57}\text{Ni} & \quad ^{58}\text{Ni} & \quad ^{59}\text{Ni} & \quad ^{60}\text{Ni} & \quad ^{61}\text{Ni} & \quad ^{62}\text{Ni} & \quad ^{63}\text{Ni} & \quad ^{64}\text{Ni} \\
\text{fraction} & \quad .0 & \quad .0 & \quad .6827 & \quad .0 & \quad .2790 & \quad .0113 & \quad .0359 & \quad .0 & \quad .0091 \\
\end{align*}

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 \textit{11670 isotopic lines}. Hyperfine splitting was included for ^{61}\text{Ni} 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

$^{59}$Co 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 | E1 lines | 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     | ...   |
| Ga  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Ge  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| As  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Se  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Br  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Kr  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Rb  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Sr  | .05   |       |       |       |       |       |       |       |       |       |
| Y   | .7    | .05   |       |       |       |       |       |       |       |       |
| 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    | 5     | ...   |
| Sb  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Te  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| I   | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Xe  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Cs  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |
| Ba  | .1    | .03   | .6    | 4     | 10    | 7     | 10    | 14    | 5     | ...   |

TOTAL 3d > 500 MILLION
TOTAL 4d > 500 MILLION
+ LANTHANIDE SEQUENCES > 1000 MILLION
+ ALL THE OTHER ELEMENT SEQUENCES
**TiO and H$_2$O**

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 $^{46}$Ti$^{16}$O, $^{47}$Ti$^{16}$O, $^{48}$Ti$^{16}$O, $^{49}$Ti$^{16}$O, $^{50}$Ti$^{16}$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 H$_2$O semiempirically. They included isotopomers H$_2^{16}$O, H$_2^{17}$O, H$_2^{18}$O, and HD$^{16}$O. 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 Vturb.

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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