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# Including All the Lines

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**Abstract.** Of the line data on my website, 99 per cent have predicted wavelengths and can be used only to compute opacities. One percent have good wavelengths between known levels and can be used for detailed spectrum calculations for comparision to observed spectra. The line data with good wavelengths account for only one half of the observed lines. The gf values and damping constants for most lines must be adjusted to match observed spectra. We know that the higher configurations are missing from the line lists. We know that heavier elements are missing from the line lists. We know that isotopic and hyperfine splittings are missing from the line lists. We know that many molecules are missing from the line lists. Leaving out all these lines systematically underestimates the opacity, produces energy distributions with systematic errors, and leads to abundance determinations with large systematic errors.

We need much better laboratory analyses including hyperfine and isotopic splitting. We need better calculations that fill in the higher configurations and the heavier elements. We need better measurements and calculations for all the significant diatomic and polyatomic molecules including all the isotopomers.

I am doing as much as I can to fill in the missing data and to make it available on my web site.

**Key words.** Stars: atmospheres – Stars: abundances – Atmospheric effects – Atomic data – Molecular data – Techniques: spectroscopic

## 1. Introduction

Half the lines in the solar spectrum are not identified. All the features are blended. Most features have unidentified components that make it difficult to treat any of the identified components in the blend. And even the known lines have hyperfine and isotopic splittings that have not yet been measured. Is an asymmetry produced by a splitting, or by a velocity field, or both? It is very difficult to determine abundances, or any property, reliably when you do not know what you are working with. Figure 1 illustrates these points. It shows one of the emptiest regions in the visible in a high-resolution, high-signal-to-noise solar spectrum taken by James Brault with the FTS at Kitt Peak together with the spectrum calculated with SYNTHE. Figure 2 is a sample section of the spectrum of Sirius observed by Glenn Wahlgren with the Goddard High Resolution Spectrograph on the Space Telescope together with the calculated spectrum.

[Fig. 1 is a large color ledger page on the Kurucz website KURUCZ.HARVARD.EDU/ PAPERS/TRIESTELINES/FIG1. It will be mailed by post on request.]

**Fig. 1.** A small section of the solar flux spectrum at 599nm plotted at full scale and at 10-times scale. The heavy black lines show the observed spectrum from the Kitt Peak Solar Flux Atlas from 300 to 1000 nm (Kurucz 2005). The resolving power is about 300000 and the signal-to-noise is about 3000. Higher quality spectra would be helpful because the spectrum is not resolved and because weaker features would appear at higher signal-to-noise.

The thin lines are the computed spectra: in red for the solar flux, in blue for the telluric atmospheric transmission, and in purple for their product which should be compared to the observed heavy black lines. The computed spectra are broadened to resolving power 0.05666 $cm^{-1}$ to match the observed spectrum. There are solar lines of Ca I, Ti I, Cr I, Cr II, Fe I, Fe II, Co I, Yb II, $C_2$, CN, and telluric lines of $H_2O$. The first number in each line label is the last 3 digits of the wavelength. The second number is the species code which is the atomic number plus 0.01 times the charge. The middle numbers are either the lower energy level in $cm^{-1}$ for atoms or quantum numbers for molecules. The 4th number is the per mil line depth if the line were computed in isolation. Two of the Co I lines have been divided into hyperfine components. The hyperfine and isotopic splittings have not yet been determined for the other lines. Some splittings may be negligible. There are many missing lines. The lines that are present have been adjusted to improve agreement between the calculated and observed spectra. That process is continuing. This sample will be part of a forthcoming flux atlas with line identifications.

[Fig. 2 is a large color ledger page on the Kurucz website KURUCZ.HARVARD.EDU/ PAPERS/TRIESTELINES/FIG2. It will be mailed by post on request.]

**Fig. 2.** A sample section of the spectrum of Sirius at 200 nm observed by Glenn Wahlgren with the Goddard High Resolution Spectrograph on the Space Telescope together with a calculated spectrum that has not yet been adjusted to improve the fit.

The rotation velocity is known from fitting lines in the visible observed at high resolution. The spectrum is computed both at 0 km/s rotation velocity to resolve the blends and at 16 km/s. The 16 km/s spectrum was then convolved with the instrumental profile. The resolution was not high enough to resolve the actual structure in the spectrum which is on the order of the zero rotation line width. Around 201.26 for example the two side bumps are washed out. Ideally the measurement should have been made at higher resolution.

The calculations are plotted in residual flux but the continuum level for the observed spectrum has not been set and its position can be adjusted. Except at 201.02 nm it appears that the observed spectrum should be moved up about 3%. That would also bring the minima into better agreement. Either the Mn II line at 201.0259 is wrong or there is a problem with the reduction at this point which is near the end of a scan. Note that the minima in the spectrum at 201.1, 201.22, and 201.42 are not line positions. Features in spectrum are blends of many lines.

Note the Si II line at 201.5 that is computed very much too strong. That will be corrected in my next calculation for Si II. Note the missing line at 201.11. That will probably appear when I recompute the Fe group lines using improved laboratory analyses. The linelist for this spectrum has not been updated with new calculations. It uses the linelist from my web site. I am going to update many elements at once to limit the number of versions of the linelist and also to give me more time to make comparisons and to check for errors. Fresh calculations can be found on the website in the /ATOMS directory.

For planetary and telluric atmosphere projects the solar irradiance spectrum is required as the input at the top of the atmosphere. It has never been observed. People ask me to compute it. I can compute it theoretically using both known and predicted lines and get agreement averaged over a nanometer but there is no way to predict the resolved spectrum when only half the lines are known. In other stars the situation is worse because the signal-to-noise and resolution of the observations are worse. Logically one has to know a priori what is in the spectrum in order to interpret it; there is not enough information in the observed spectrum itself.

Basically we need a list of all the energy levels of all atoms and molecules that matter (qualifiers below). From that list can be generated all the lines. With the energy levels and line positions known, one can measure gf values, lifetimes, damping, or one can determine a theoretical or semiempirical Hamiltonian whose eigenvalues and eigenvectors produce a good match to the observed data, and that can then be used to generate additional radiative and collisional data for atoms or molecules. Forbidden magnetic dipole and electric quadrupole lines are required as well.

For atoms and ions, we need all levels, including hyperfine and isotopic splittings, for n $\leq$ 9 below the lowest ionization limit and as much as practicable above. Lifetimes and damping constants depend on sums over the levels.

Radiative acceleration in stellar envelopes can selectively levitate some elements. At the visible surface the enhancement can be as much as a factor of $10^4$. The radiative acceleration is computed by integrating $l_\nu J_\nu$ over the spectrum. If the diffusion takes place deep in the envelope, spectra for high stages of ionization are required. For heavier elements we need at least the first 5 stages of ionization.

In the sun I see unidentified asymmetric triangular features that are unresolved multiplets of light elements with n $\leq$ 20. Simple spectra should be analyzed up to n = 20. Levels that connect to the ground or to low levels should be measured to high n, say n = 80. The high levels are necessary to match line series merging into continua.

For molecules, we need all levels below the first dissociation limit and as much as is practicable above, especially levels of all states that connect to the ground state. Except for $H_2$(BX,CX), far ultraviolet bands have been ignored unless they appear as interstellar lines. We see $H_2$ lines in stars as hot as 8000K when the stars have low metal abundances so that the lines are not masked.

In the sun we see, and have line lists for,
$C_2$(AX,ba,da,ea),
CN(AX,BX),
CO(AX,XX),
$H_2$(BX,CX),
CH(AX,BX,CX),
NH(AX,ca),
OH(AX,XX),
MgH(AX,BX),
SiH(AX),
SiO(AX,EX,XX).
The isotopomers are included. Some stellar spectroscopists have more recent linelists than I do. Mine are based on old laboratory data and were computed with rotationless RKR potentials. They all have to be brought up to date, or even further improved, and expanded to higher V and J levels. In many cases there are new analyses based on FTS spectra. Ions and a few minor molecules have to be added to the linelist as well. In the sun there are many broad bumpy unidentified features that are molecular bands that are not in the line lists. Most of them are probably just high-V transitions. It is important that the laboratory analyses include all the isotopomers. They are needed to interpret the stellar spectra. When they are not measured in the laboratory, we have to make up our own predicted linelists for them.

For the cooler stars we need all the diatomics among all the abundant elements, and, essentially, the hydrides and oxides for all elements (such as ScO. TiO, VO, YO, ZrO, LaO, etc.). Ca appears as CaOH and CaH, not CaO. I use the TiO linelist from Schwenke (1998) with 38 million lines.

Stars that are evolved and have high C abundances from nuclear burning can bind all the O into CO so that there are no other oxides, just C-bearing molecules. CN and $C_2$ bands are everywhere.

For M stars cooler than 3500K triatomics also become important. Much more laboratory and computational work is needed for $H_2O$. I currently use the linelist from Partridge and Schwenke (1997) with 66 million lines.

In the brown dwarfs and "planets" methane is important and it needs more laboratory and computational work.

Some of this is described in more detail in my paper "Atomic and molecular data needs for astrophysics" (Kurucz 2002, on Kurucz website).

## 2. Adding atomic and molecular data

The basic rule seems to be that if you need data you have to produce it yourself. My workstation and my website have a directory for each ion of all the atoms up through Zn, and the first five ions of heavier elements, and for all the diatomic molecules that I should work on.

Here is the background starting with my calculations at the San Diego Supercomputer Center in the 1980s. I have computed line data for 42 million lines of the iron group elements (Kurucz 1988) plus I have all the data from the literature for all elements (but I am not current). I have computed line data for 16 million diatomic molecular lines. (Some as much as 20 years ago.) They are the basic data for computing opacoties and spectra. Only 1 per cent (i.e., 600,000) of my computed lines have accurate wavelengths between known levels because the laboratory analyses have not yet found the levels and need improvement. When published theory or laboratory f values or broadening data seem better than mine, I use the better data. This "good" line list is the input for spectrum synthesis programs. I put the line data on my web site, KURUCZ.HARVARD.EDU, as they are produced.

I have added the TiO and $H_2O$ line lists from Schwenke and I have thrown out my old TiO linelist. That leaves me with 154 million lines with which I can compute reasonable models for M stars down to 3500K.

To compute the iron group line lists I made Slater-expansion model Hamiltonians that included as many configurations as I could fit into the Cray. I used Hartree-Fock Slater integrals (scaled) for starting guesses and for higher configurations that had no laboratory energy levels. All configuration interactions were included. I then determined the Slater integrals for the observed configurations by least squares fitting the eigenvalues computed from the Hamiltonian matrix to the observed energies. The complication was that the eigenvalues and the observed energies had to be correlated by hand each iteration and more than a hundred interations were often required for convergence. My computer programs for these procedures have evolved from Cowan's (1968) programs. Transition integrals were computed with scaled-Thomas-Fermi-Dirac wavefunctions and the whole transition array was produced for each ion. Radiative, Stark, and van der Waals damping constants and Landé g values were automatically produced for each line. The first nine ions of Ca through Ni produced 42 million lines. Eigenvalues were 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.

I am now computing or recomputing all the atoms and diatomic molecules. My old Cray programs from the 1980s were limited to 1100 x 1100 arrays in the Hamiltonian for each J. With my Alpha workstation I can easily run cases with 3000 x 3000 arrays so that I can include many more configurations and many more configuration interactions. The larger arrays produce about 3 times as many lines. At present I am limited to 61 even and 61 odd configurations and

I try to include everything up through n = 9. I give examples below that illustrate various improvement in the new calculations.

In section 4 I show statistics from my new semiempirical calculations for Fe II, Ni I, Co I, C I, and S 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 to 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. 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. Laboratory measurements of gf values and lifetimes will be included.

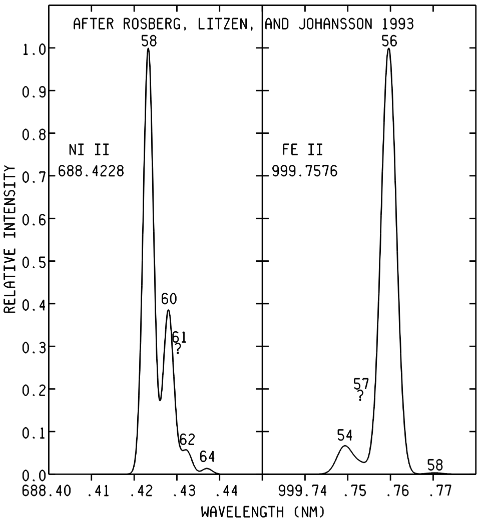


**Fig. 3.** Examples of isotopic splitting in Fe II and Ni II after Rosberg, Litzén, and Johansson (1993). The indications for $^{61}$Ni and $^{57}$Fe are guesses.

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

## 3. Isotopic and hyperfine splitting

There are two papers on isotopic and hyperfine splitting on my website (Kurucz 1992; 1993). In the second is a table that lists all the stable isotopes, their fractional abundances, nuclear spin, dipole moment, and quadrupole moment. The only element that does not have isotopic or hyperfine splitting is thorium. "Lines" are normally asymmetric because of the splitting. Figure 3 from Rosberg, Litzen, and Johansson (1992) show the isotopic splitting of an Fe II line and a Ni II line. If the splitting is not taken into account many kinds of errors are possible: the use of bisectors to determine velocity fields is incorrect; Fourier analysis of line profiles to determine rotational, microturbulent, and macroturbulent velocities is incorrect; damping constants are over-estimated. When stronger components become saturated, the weak compo-

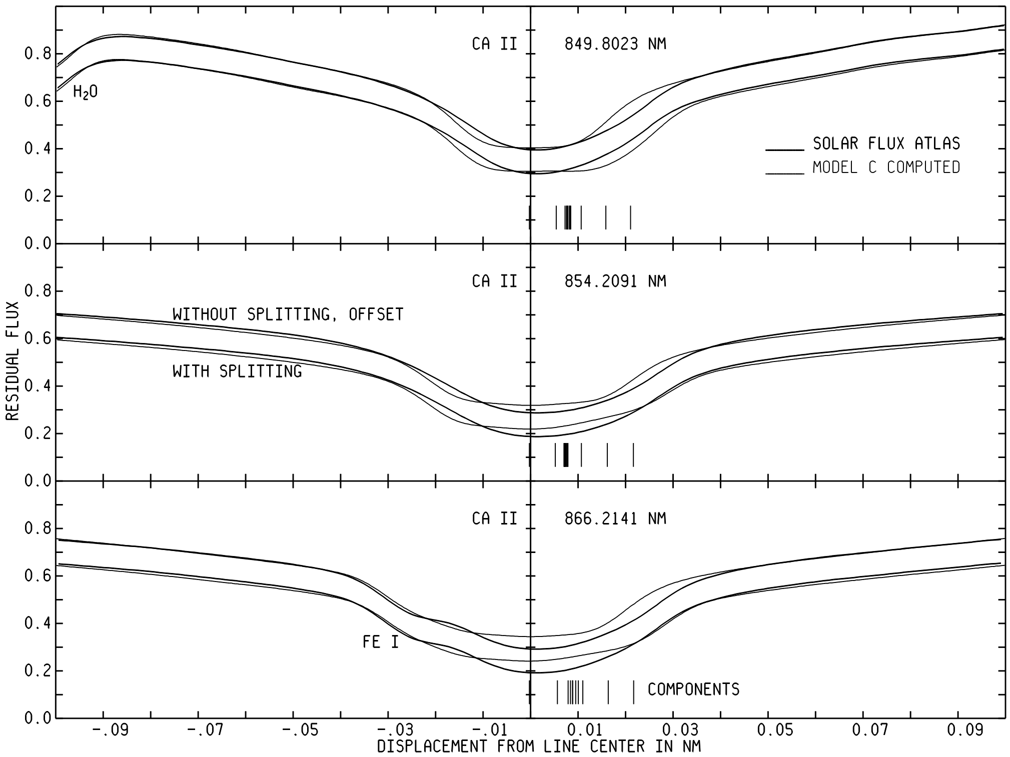


**Fig. 4.** Asymmetries in the Ca II infrared triplet arise from isotopic and hyperfine splittings, not from velocity or non-LTE effects. The splitting data are listed in Table 1. Two Å around each line are plotted twice, centered on the centroid wavelength, with splitting, and, offset, without splitting. The calculation uses model C by Fontenla, Avrett, and Loeser 1993 which has a chromosphere. In lieu of a real non-LTE calculation, the line opacity was smoothly changed to scattering for $\tau_{Ross} < 0.04$. The number was chosen by experimenting until the emission from the chromosphere was eliminated. Note that the splitting also changes the line wings. The heavy lines are the observed spectrum from the Kitt Peak Solar Flux Atlas from 300 to 1000 nm (Kurucz 2005).

nents are still on the linear part of the curve of growth. They make a larger contribution to the total feature than their fractional abundances might suggest. This introduces the additional systematic errors: wavelengths of saturated lines are shifted relative to the isotopic abundance weighted position; abundances determined from equivalent widths are wrong unless the curve of growth is computed from the real line profile with components. In addition, the Doppler width and Voigt profile differ significantly from the lightest to the heaviest isotope.

I was recently asked about the Ca II infrared triplet so I collected the data from the literature. Figure 4 shows the solar flux spectra for the cores of the Ca II infrared triplet lines for two Å around their centroid wavelengths and with the LTE computed profiles including hyperfine and isotopic splitting. In non-LTE the cores become weaker as observed. The components are listed in Table 1.

Molecular lines can also have hyperfine splitting, but I have not yet had to deal with it.

**Table 1. Hyperfine and isotopic splitting for the Ca II infrared triplet.**

Centroid data from KURUCZ.HARVARD.EDU/LINELISTS/GFALL/GF2001.ALL

| wl(nm) | loggf | ref | E | J | label | E′ | J′ | label′ | gamr | gams | gamw | glande | glande′ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 849.8023 | -1.312 | BWL | 13650.190 | 1.5 | 3d 2D | 25414.400 | 1.5 | 4p 2P | 8.20 | -5.55 | -7.80 | 0.800 | 1.334 |
| 854.2091 | -0.362 | BWL | 13710.880 | 2.5 | 3d 2D | 25414.400 | 1.5 | 4p 2P | 8.20 | -5.55 | -7.80 | 1.200 | 1.334 |
| 866.2141 | -0.623 | BWL | 13650.190 | 1.5 | 3d 2D | 25191.510 | 0.5 | 4p 2P | 8.19 | -5.55 | -7.80 | 0.800 | 0.666 |

Hyperfine A and B for 43Ca II, spin I 3.5

| E | J | label | A(MHz) | B(MHz) | ref |
|---|---|---|---|---|---|
| 0.000 | 0.5 | 4s 2S | -797.5 | 0.0 | GM |
| 13650.190 | 1.5 | 3d 2D | -52. | -4.42 | MPS |
| 13710.880 | 2.5 | 3d 2D | -5.2 | -6.305 | MPS |
| 25191.510 | 0.5 | 4p 2P | -158.0 | 0.0 | GM |
| 25414.400 | 1.5 | 4p 2P | -30.9 | -10.1 | MPS |

Isotopic splitting from MP (46 and 48 extrapolated)

| wl(nm) | iso | log hyper f | log iso frac | F F′ | hfshift dE(mK) | dE′ | isoshift (mA) |
|---|---|---|---|---|---|---|---|
| 849.8020 | 40 | 0.000 | -0.013 | | 0 | 0 | -3 |
| 849.8077 | 42 | 0.000 | -2.189 | | 0 | 0 | +54 |
| 849.8095 | 43 | -1.017 | -2.870 | 5-4 | -9 | 0 | +78 |
| 849.8098 | 43 | -0.903 | -2.870 | 4-3 | 0 | 4 | +78 |
| 849.8099 | 43 | -0.606 | -2.870 | 5-5 | -9 | -5 | +78 |
| 849.8101 | 43 | -1.028 | -2.870 | 3-2 | 7 | 7 | +78 |
| 849.8101 | 43 | -1.222 | -2.870 | 4-4 | 0 | 0 | +78 |
| 849.8105 | 43 | -1.204 | -2.870 | 2-2 | 12 | 7 | +78 |
| 849.8105 | 43 | -1.017 | -2.870 | 4-5 | 0 | -5 | +78 |
| 849.8106 | 43 | -0.903 | -2.870 | 3-4 | 7 | 0 | +78 |
| 849.8107 | 43 | -1.028 | -2.870 | 2-3 | 12 | 4 | +78 |
| 849.8129 | 44 | 0.000 | -1.681 | | 0 | 0 | +109 |
| 849.8181 | 46 | 0.000 | -4.398 | | 0 | 0 | +161 |
| 849.8233 | 48 | 0.000 | -2.728 | | 0 | 0 | +213 |
| | | | | | | | |
| 854.2088 | 40 | 0.000 | -0.013 | | 0 | 0 | -3 |
| 854.2143 | 42 | 0.000 | -2.189 | | 0 | 0 | +52 |
| 854.2161 | 43 | -1.204 | -2.870 | 2-2 | 2 | 7 | +74 |
| 854.2161 | 43 | -1.505 | -2.870 | 3-2 | 1 | 7 | +74 |
| 854.2162 | 43 | -1.204 | -2.870 | 1-2 | 2 | 7 | +74 |
| 854.2163 | 43 | -1.380 | -2.870 | 2-3 | 2 | 4 | +74 |
| 854.2163 | 43 | -1.040 | -2.870 | 3-3 | 1 | 4 | +74 |
| 854.2163 | 43 | -1.066 | -2.870 | 4-3 | 0 | 4 | +74 |
| 854.2165 | 43 | -0.783 | -2.870 | 5-4 | 0 | 0 | +74 |
| 854.2166 | 43 | -1.630 | -2.870 | 3-4 | 1 | 0 | +74 |
| 854.2166 | 43 | -1.032 | -2.870 | 4-4 | 0 | 0 | +74 |
| 854.2168 | 43 | -0.567 | -2.870 | 6-5 | -2 | -5 | +74 |
| 854.2169 | 43 | -2.058 | -2.870 | 4-5 | 0 | -5 | +74 |
| 854.2169 | 43 | -1.193 | -2.870 | 5-5 | 0 | -5 | +74 |
| 854.2198 | 44 | 0.000 | -1.681 | | 0 | 0 | +107 |
| 854.2252 | 46 | 0.000 | -4.398 | | 0 | 0 | +161 |
| 854.2307 | 48 | 0.000 | -2.728 | | 0 | 0 | +216 |

| wl(nm) | iso | log hyper f | log iso frac | F F′ | hfshift dE(mK) | dE′ | isoshift (mA) |
|---|---|---|---|---|---|---|---|
| 866.2138 | 40 | 0.000 | -0.013 | | 0 | 0 | -3 |
| 866.2197 | 42 | 0.000 | -2.189 | | 0 | 0 | +54 |
| 866.2220 | 43 | -0.931 | -2.870 | 4-3 | 0 | 12 | +78 |
| 866.2225 | 43 | -0.785 | -2.870 | 3-3 | 7 | 12 | +78 |
| 866.2229 | 43 | -0.806 | -2.870 | 2-3 | 12 | 12 | +78 |
| 866.2229 | 43 | -0.464 | -2.870 | 5-4 | -9 | -9 | +78 |
| 866.2236 | 43 | -0.785 | -2.870 | 4-4 | 0 | -9 | +78 |
| 866.2241 | 43 | -1.262 | -2.870 | 3-4 | 7 | -9 | +78 |
| 866.2251 | 44 | 0.000 | -1.681 | | 0 | 0 | +109 |
| 866.2304 | 46 | 0.000 | -4.398 | | 0 | 0 | +163 |
| 866.2358 | 48 | 0.000 | -2.728 | | 0 | 0 | +217 |

GM Goble, A.T. and Maleki, S. 1990, Phys. Rev. A 42, 649-650.

MPS Martensson-Pendrill, A. and Salomonson, S. 1984. Phys. Rev. A 30, 712-721.

MP Martensson-Pendrill,A-M., Ynnerman, A., et al. 1992. Phys. Rev. A 45, 4675-4681.

## 4. Examples

### *4.1. Fe II*

The semiempirical calculation for n$\leq$9 was based on Johansson (1978) and on more recent published and unpublished data. Johansson has data for more than 100 energy levels that I do not yet have. There were 46 even configurations: $d^7$, $d^6$ns, nd, ng, ni, nl, $d^5$4sns, nd, ng, ni, nl, $d^4 4s^2$4d, $d^4 4s^2$5s, $d^5 4p^2$ which produce 19771 levels of which 403 are known. There are 39 odd configurations: $d^6$np, nf, nh, nk, $d^5$4snp, nf, nh, nk, $d^4 4s^2$4p, $d^4 4s^2$5p, $d^5 4s^2$4f, which produce 19652 levels of which 492 are known. These produced 7,719,963 E1 lines and 28 million M1 and E2 lines. Only 81225 E1 lines have good wavelengths. Only 2884 of the forbidden lines are from metastable levels. The previous calculation (Kurucz 1988) produced 1,264,969 lines with 45815 good wavelengths. There are four stable isotopes:

Isotopes $^{54}$Fe $^{56}$Fe $^{57}$Fe $^{58}$Fe

| | | | | |
|---|---|---|---|---|
| Fraction | .059 | .9172 | .021 | .0028 |

Only a few lines have been measured by Rosberg, Litzén, and Johansson (1993) so I put in the splittings by hand.

### 4.2. Ni I

The Ni I calculation was mostly based on the analysis by Litzén, Brault, and Thorne (1993) which includes isotopic splitting. There were 46 even configuations with 3203 levels of which 120 are known. There were 48 odd configurations with 4800 levels of which 153 are known. These produced 529632 E1 lines compared to 149926 from Kurucz (1988). Only 9637 lines have good wavelengths. There were 1.5 million M1 and E2 lines of which 65 were from metastable levels. There are 5 stable isotopes,

| Isotope | $^{58}$Ni | $^{60}$Ni | $^{61}$Ni | $^{62}$Ni | $^{64}$Ni |
|---|---|---|---|---|---|
| Fraction | .6827 | .2790 | .0113 | .0359 | .0091 |

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 $^{61}$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. When the isotopic calculation was first checked against the solar spectrum it did not look right. Subsequently, I found a program error and recomputed the splittings. Now the profiles match the observed. Observed stellar spectra are generally not high enough quality to show that there are such errors.

### 4.3. Co I

The Co I calculation was based on Pickering and Thorne (1996) and on Pickering (1996) with hyperfine splitting. This calculation was made before my programs were expanded. I will rerun this with twice as many configurations. This calculation had 32 even configurations with 3546 levels of which 139 were known. There were 32 odd configurations with 5870 levels of which 223 were known. These produced 1729299 E1 lines of which 15481 were between knowm levels. The old calculation (Kurucz 1988) produced 546130 lines. There were 4.7 million forbidden lines of which 696 were from metastable levels, $^{59}$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.

### 4.4. C I

The lower levels of C I were computed as in the previous examples and higher levels up to n = 20 were added from Ritz extrapolation for low l or from the polarization formula for high l. There were 136 even configurations: s$^2$p$^2$, s$^2$pnp, nf, nh, nk, nm, no, nr, nv, nw, ny, with 2382 levels. There were 139 odd configurations: s$^2$pns, nd, ng, ni, nl, nn, nq, nt, nv, nx, sp$^2$np, p$^3$ns, p$^3$nd, with 1962 levels. They produced 469918 E1 lines of which 182979 have good wavelengths. The low levels produced 652897 forbidden lines of which 10 were from metastable levels. The series were extrapolated to n = 99 to produce 36182 lines that merge into low continua. I have not yet worked on the isotopic or hyperfine splitting. The isotopes are 0.9890 $^{12}$C and 0.0110 $^{13}$C.

I am now doing Si I in the same way.

### 4.5. S I

There were 61 even configuarations with 2161 levels and 61 odd configuartions with 2270 levels. They produced 225605 E1 lines of which 24722 had good wavelengths. I have added measured autoionization parameters to the ultraviolet lines by hand. There are 4 stable isotopes,

| Isotopes | $^{32}S$ | $^{33}S$ | $^{34}S$ | $^{36}S$ |
|---|---|---|---|---|
| Fraction | .9502 | .0075 | .0421 | .0002 |

I have not yet worked on the isotopic or hyperfine splitting.

### 4.6. TiO

Schwenke (1998) 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 (1998) transition moments Schwenke generated a linelist for J = 0 to 300 for the

| Isotopomers | $^{46}TiO$ | $^{47}TiO$ | $^{48}TiO$ | $^{49}TiO$ | $^{50}TiO$ |
|---|---|---|---|---|---|
| Fraction | .080 | .073 | .738 | .055 | .054 |

My version has 37744499 lines.

### 4.7. Oxides

Good laboratory analyses and a semiempirical treatment similar to that for TiO are needed for CaOH, ScO, VO, YO, ZrO, LaO, etc. Better laboratory data could be used to further improve TiO.

## 5. References

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