SYNTHETIC INFRARED SPECTRA

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Abstract. The Sun is the star we can observe with the highest spectral resolution and signal-to-noise. From studying the infrared spectrum we can learn about the Sun, about stars in general, and about atomic and molecular spectroscopy. We discuss the computer programs for spectrum synthesis, the infrared flux and central intensity atlases of the solar spectrum, and the atomic and molecular line data. Considerable work is still required to improve the observations and to improve the line data.

Key words: atomic data – infrared: stars – line: formation – molecular data – Sun: atmosphere

1. The Importance of Studying the Solar Spectrum

The spectrum of a star consists of many thousands of lines blended together. Even at infinite resolution and signal-to-noise the blends are difficult to interpret. At low resolution and signal-to-noise a spectrum does not contain enough information for interpretation. Without a priori information from other sources, the analysis of such a spectrum is usually incorrect. I believe that we can learn more by studying the brightest stars with the highest possible resolution and signal-to-noise, than from any number of poor observations of fainter stars.

The Sun is the brightest star available to us. It is possible to observe the solar spectrum with a signal-to-noise of 10^4 and a resolving power of 10^6; but nobody has. In the Sun we can study contributions to blends at the 1 per mil level. Such lines can be better observed in the Sun than lines that are 1000 times stronger in a globular cluster star. There are many cases where lines can be seen in the Sun that have been difficult or impossible to see in the laboratory. The Sun is a unique spectroscopic source for studying atoms and molecules. Below I discuss the solar atlases that are available, but there is very little compared to what could be easily obtained, and there is very little compared to what is needed.

I have developed computer programs for producing model stellar atmospheres and for synthesizing spectra. I am collecting and computing data on all relevant atomic and molecular lines. I check the line gf values and damping constants by comparing the computed spectra to the observed spectra. Once I can compute realistic spectra for the Sun and the brightest stars these programs and data can be used to predict the spectra of stars that are too faint to observe well (or even stars from the early universe that no longer exist). Below I discuss these computer programs and the line data.

2. Spectrum Synthesis Programs

The spectrum synthesis computer programs have been under development since 1965 and have been described by Kurucz and Furenlid (1981) and by Kurucz and Avrett (1981). The algorithms for computing the total line opacity are extremely fast because maximum use is made of temperature and wavelength factorization and pretabulation. On a Cray computer a 500,000 point spectrum can be computed in

one run. The same programs run on a VAX, only much more slowly. There is no limit to the number of spectrum lines that can be treated in LTE. I currently have 58,000,000. At present I can treat 50,000 lines including non-LTE effects. The line data are described below.

The spectrum calculations require a pre-existing model atmosphere that can be empirical, such as the Vernazza, Avrett, and Loeser (1981) solar models, or theoretical, such as the ones I describe below. The "model atmosphere" does not have to be stellar. It can be a disk, a planetary atmosphere, a laboratory source, etc. Quantities that need be computed only once for the model atmosphere are pretabulated. There can be a depth-dependent microturbulent velocity or a depth-dependent Doppler shift.

Line data are divided into two groups for treatment. In the first group, the lines must have a source function that is either the Planck function or some function that approximately accounts for non-LTE effects in the outer layers. The first group of lines is processed to produce a summed line absorption coefficient for the wavelength interval of interest, including radiative, Stark, and van der Waals broadening. The line center opacity is also saved for each line for subsequent computation of the central depth.

In the second group of lines, each line has its individual source function, which is taken to be the Planck function if the calculation is LTE, and which is determined from the departure coefficients in the model in a non-LTE calculation. This group of lines is processed by directly computing the line opacity and source function at every wavelength point.

The spectrum is computed with a version of the model atmosphere program ATLAS (Kurucz 1970) in which departure coefficients have been inserted in the partition functions, in the Saha and Boltzmann equations, and in the opacities. Departure coefficients for levels that are higher than have been computed are assumed to be the same as those for the ground state of the next higher stage of ionization. If the model atmosphere is in LTE the departure coefficients are all set to unity. The program computes the non-LTE opacity and source function, adds in the LTE opacity and source function, adds the continuum opacity and source functions, and then computes the intensity or flux at each wavelength point and for each line center. Photoionization continua are put in at their exact positions, each with its own cross-section and with the series of lines that merge into each continuum included so that there are no discontinuities in the spectrum.

Hydrogen line profiles are computed using a routine from Peterson (1979) that approximates the Vidal, Cooper, and Smith (1973) profiles, works to high n, and includes Doppler broadening, resonance broadening, van der Waals broadening, and fine-structure splitting. Autoionization lines have Shore-parameter Fano profiles. Other lines have Voigt profiles that are computed accurately for any value of the parameter a. A few strong lines can be treated with approximate partial redistribution effects but the computer cost increases dramatically.

To compute a rotationally broadened flux spectrum I first compute intensity spectra at 17 angles and then pass them through the rotation program. A grid of points is defined on the disk and, for the given $v \sin i$, the Doppler shift and angle are computed for each point. The intensity spectra are interpolated and summed over

the disk to obtain the flux. In the rigid-body spherical approximation, symmetries are used to reduce the number of calculations, but the method works in the case of differential rotation as well.

To compute macroturbulent or instrumental broadening the broadening function is defined at integral values of the point spacing. Then the spectrum is read in, one wavelength at a time, redistributed among neighboring wavelengths, and added to a buffer for the new spectrum.

I also have a series of programs for computing the transmission of the spectrum through the Earth's atmosphere using the HITRAN database (Rothman *et al.* 1987) for the line data.

The most important step in the spectrum synthesis work is the final preparation of plots because I can display enough information to study the spectrum as a whole, to compare with one or more observed spectra, to study individual features in detail, and to identify lines and the relative composition of blends. Figures 1 and 2 show small sections of spectrum selected because they do not show dramatic discrepancies between the calculated and observed spectra. The figures show raw calculations, without adjustment. Usually the fits are much worse, with many missing lines.

3. Atlases

I have made a considerable effort to obtain observed spectra of the Sun and bright stars for testing my calculations. I have all the published atlases. Fortunately, Delbouille and Roland and the Griffins are committed to producing high quality atlases for the Sun and for bright stars, respectively. I have many solar FTS spectra from James Brault at Kitt Peak. In many cases I have had to take or reduce the spectra myself (Kohl, Parkinson, and Kurucz 1978; Kurucz and Avrett 1981; Kurucz and Furenlid 1981; Kurucz, Furenlid, Brault, and Testerman 1984), and projects are now underway for Sirius, Vega, and the Sun with a number of collaborators. Here I will describe a few of these atlases to give an impression of what is available in the infrared. In every case the wavelength coverage is incomplete and higher quality is possible and needed. I have a review paper (Kurucz 1992a) that shows each solar atlas plotted at very reduced scale.

The solar flux spectrum is important for its effects on atmospheric chemistry, on solar system objects, and on us, rather than for solar physics. In the flux spectrum much of the spatial and Doppler information about the solar atmosphere has been integrated away leaving a spectrum broadened and blended by the 2 km s^{-1} solar rotation. The flux spectrum is quite important for stellar physics, however, because the Sun serves as the "standard star". We can determine its properties much better than those of any other star. Solar flux spectra are required for planning and interpreting stellar and planetary observations because they have the resolution and signal-to-noise to show what is actually being observed.

As observations made from ground-based observatories include the atmospheric transmission spectrum, it is necessary to consider blending and blocking by terrestrial lines and to have resolution high enough to resolve their profiles. A solar flux spectrum observed from the ground is useful for indicating these problems. The spectrum should have a resolving power greater than 10^6 and a signal-to-noise
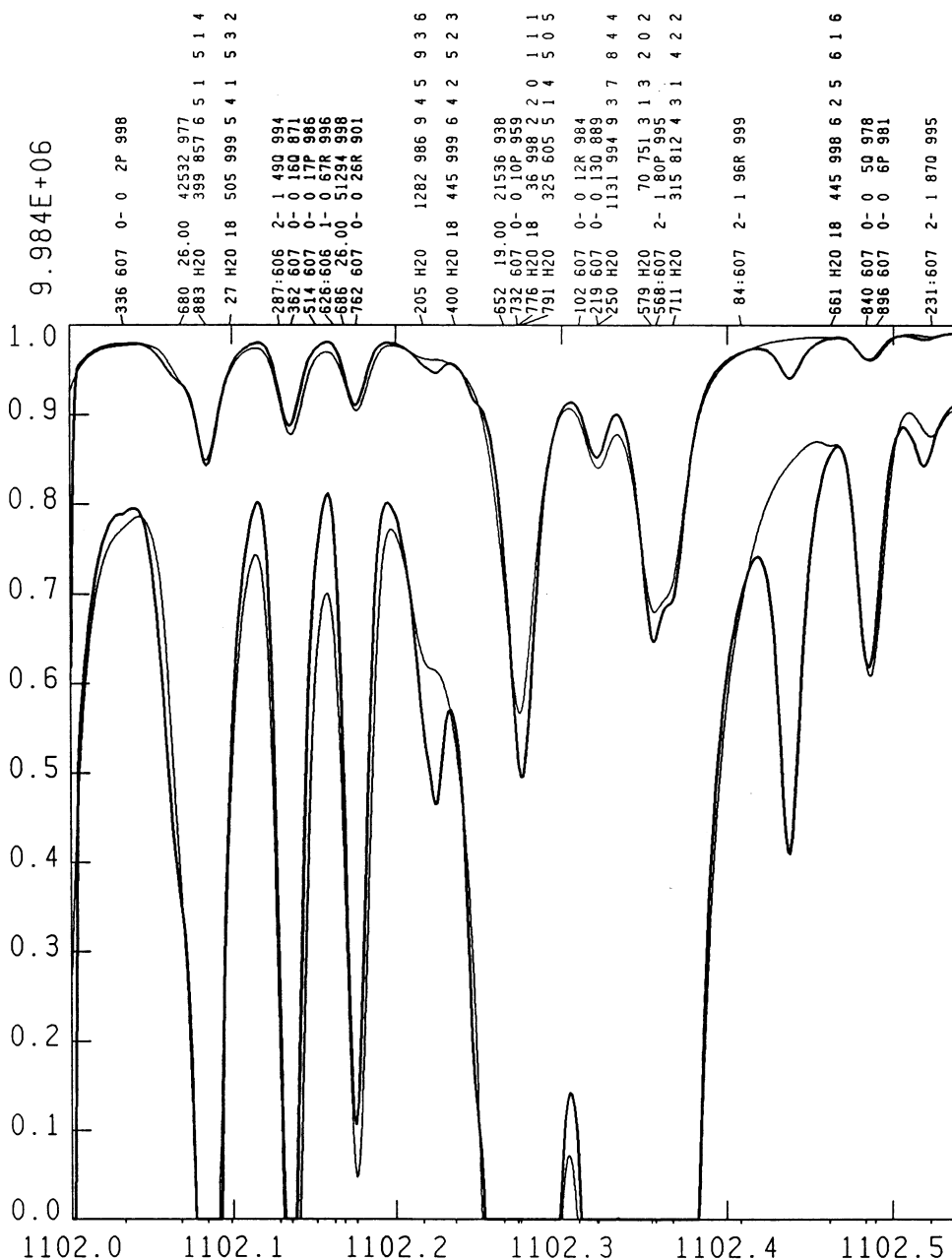
Fig. 1. A sample plot comparing a computed spectrum (thin line) to the 1.1 μm (1100 nm) central intensity spectrum observed by Brault (thick line). The spectra are shown twice, once at full scale, and once at 10 times scale. The long line labels are for terrestrial H_2O. The shorter labels are C_2, CN, Fe, and K lines. In each label the first 3 digits are the last 3 digits of the wavelength. The last 3 digits in the label are the per mil residual intensity of each line. Note the two obviously missing lines.
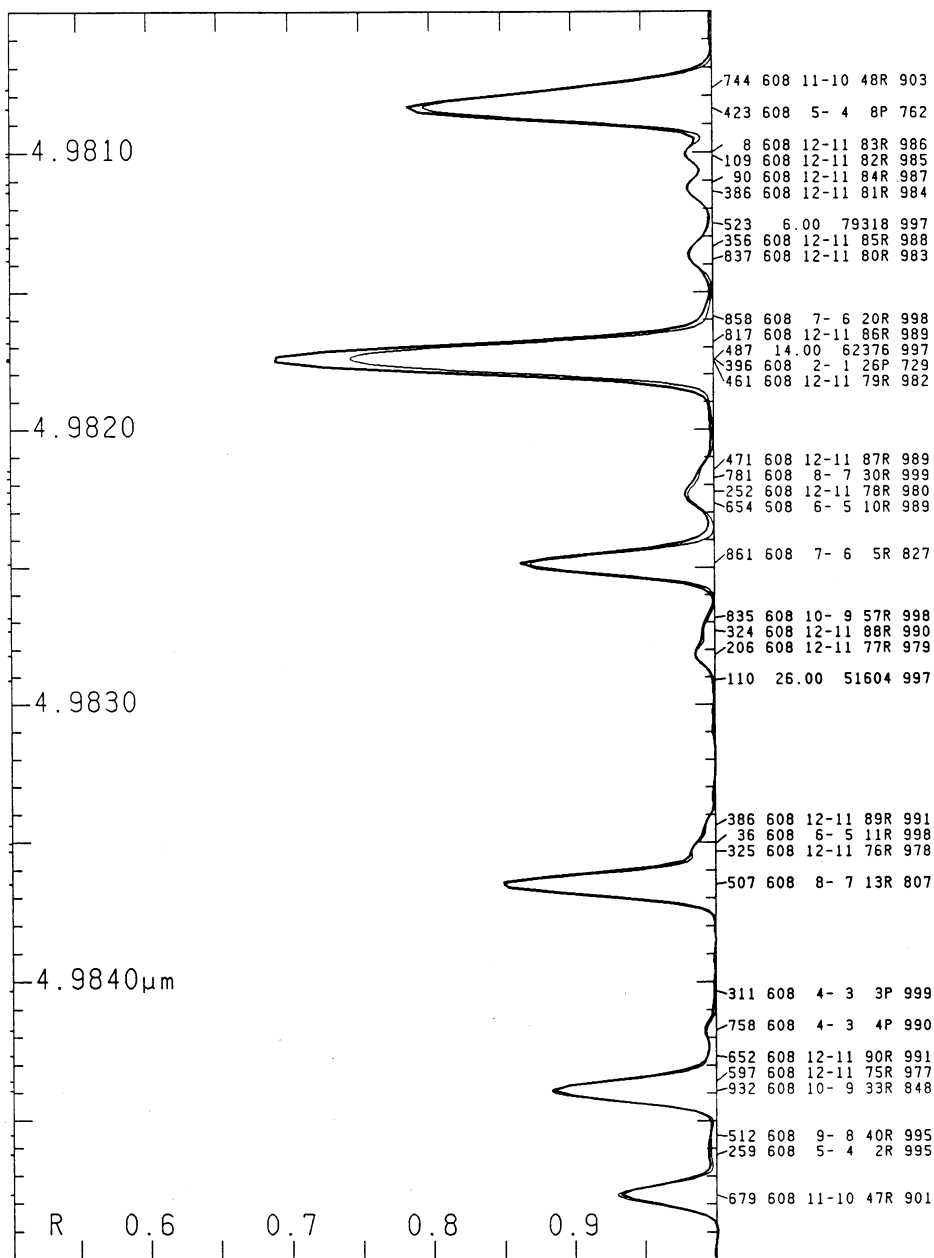
Fig. 2. A sample calculation near 5 μm (thin line) compared to the *ATMOS* central intensity spectrum described below (thick line). Except for single lines of C, Si, and Fe the lines are from highly excited bands of CO. In each label the first 3 digits are the last 3 digits of the wavelength. The last 3 digits in each label are the per mil residual intensity of each line.

greater than 10^4. For atmospheric chemistry and planetary and cometary atmospheres, and for space-based stellar observations, however, the true flux spectrum above the atmosphere is required.

The flux spectrum has been poorly observed. The existing atlas by Kurucz, Furenlid, Brault, and Testerman (1984) covers only the ground based spectrum up to 1.3 μm. It is very high quality by astronomical standards but still leaves considerable room for improvement. The atlas plots residual flux and also gives a table to convert to the absolute irradiance calibration by Neckel and Labs (1984). The spectrum was observed at Kitt Peak using the Fourier Transform Spectrograph on the McMath telescope at resolving power 522000 in the red and infrared. The resolution is not high enough to resolve the terrestrial lines so there is some ringing. The signal-to-noise varies from 2000 to 9000. The continuum level was estimated from high points and it is uncertain because of problems caused by broad structures in the atmospheric transmission produced by ozone and O_2 "dimer". In the infrared the O_2 "dimer" features are at 1.06 and 1.26 μm.

There are no high resolution flux atlases covering other wavelength regions in the infrared and there are none above the atmosphere. I do not expect there to be any improvement this century. In the meantime there are three approaches to approximating the flux spectrum. The first is to model the atmospheric transmission and then to divide the ground based spectrum by it. This should work quite well as long as the signal-to-noise is very high and the transmission is not near zero. The second method is semi-empirical: fitting a central intensity spectrum computed from a model to the observed central intensity spectrum and then using the derived line parameters to generate the flux spectrum. The problem is that a significant fraction of the lines in the spectrum have not been identified so they would have to be guessed. The third method is to compute a purely theoretical flux spectrum from the existing line data, but that is beyond the state of the art.

Intensity spectra are better for spectroscopy because there is no rotational broadening and so less blending. They are better for solar physics because they are determined by conditions in only a small region of the disk. Spectra-spectroheliograms show the spectrum at each resolution element, but they give almost too much information because they emphasize the instantaneous velocity field. The existing intensity atlases are space and time averages over a small area on the disk.

The Kitt Peak infrared central intensity atlas by Delbouille, Roland, Brault, and Testerman (1981) is the best available spectrum in the infrared. It is the combination of 9 FTS scans on the McMath telescope with resolving power about 400000 at 1 μm decreasing to about 130000 at 5 μm. The signal-to-noise varies from 3200 to 5200. Delbouille and Roland are redoing the atlas from Jungfraujoch to improve the resolution and signal-to-noise and especially to reduce the water vapor which is very bad on Kitt Peak.

Livingston and Wallace (1991) have just produced a new central intensity atlas for 1.1 to 5.4 μm with resolution 0.015 cm^{-1}. They observed at various airmasses and then reduced the spectra to 0 airmass where the atmospheric transmission was high enough to allow ratioing. They include many line identifications.

The JPL *ATMOS* experiment (Farmer and Norton 1989) was flown on the shuttle to obtain infrared FTS spectra of the atmosphere at sunset from which

to measure trace molecules. Before sunset, solar intensity spectra were recorded. Wavelength coverage is 2 to 16 μm, resolution is 0.0147 cm^{-1}, and signal-to-noise varies from 1000 to 3000. These spectra show beautiful vibration-rotation bands of CO and hydrides. The two volume atlas of Farmer and Norton (1989) shows all the solar and terrestrial data. I have obtained the data tapes, reduced them, set the continuum level, and plotted the solar data on a very expanded scale. I can supply paper or magnetic tape copies of my version.

I plan to publish or republish atlases for the Sun and bright stars with the lines labeled, including terrestrial lines from the AFGL HITRAN line list (Rothman *et al.* 1987). I am synthesizing each spectrum and should be able eventually to deconvolve the blends and to deconvolve the atmospheric transmission where it is not near zero.

4. Atomic and Molecular Data Needs

All the calculations described above depend on having reliable gf values and damping constants for atomic and molecular lines, photoionization cross-sections, and, for non-LTE problems, collision cross-sections. My work on atomic and molecular line data and my line lists are described in Kurucz 1992*b*. Here I will concentrate on the present problems and on my future work.

Accurate energy levels, accurate wavelengths, accurate gf values, and accurate damping constants are required for computing spectra. Hyperfine and isotopic splitting are also required, and for magnetic structures, Landé *g* values are needed. We require completeness because we need to deconvolve blends. We need every level below the lowest ionization or dissociation energy. For molecules, every vibrational and rotational level is needed, not just the ones populated at low temperatures in the laboratory.

The procedure I use for generating line lists is straightforward and produces all the lines up to a specified cut-off lower energy level. I start with all the known energy levels. I set up a model Hamiltonian that uses a Slater integral expansion for atoms or a rotational expansion for molecules. Then I do a least squares fit to determine the Slater integrals or the rotational constants. For atoms I use scaled Hartree-Fock starting guesses for the integrals. Once the fit has converged, I use the Hamiltonian to generate all possible eigenvalues and eigenvectors. The eigenvalues are replaced by the observed energies where they are known. For atoms I generate a scaled-Thomas-Fermi-Dirac wavefunction for each configuration and compute all the transition integrals. For molecules I compute the RKR potential and then all the vibrational wavefunctions. I then integrate over measured or computed transition moments taken from the literature to get the transition integrals. The transition integrals are divided into transition arrays in the adopted basis and are transformed to observed coupling using the eigenvectors. Given enough computer time, I can readily generate thousands of energy levels and millions of lines. Thus far I have produced atomic and molecular line lists with 58 million lines. Since the known energy levels are used when available, the line wavelengths are correct for lines between known energy levels. Lines to predicted levels are as accurate as the least squares fitting procedure. Radiative, Stark, and van der Waals damping constants

and Landé g values are automatically produced for each line.

Problems arise when not all the "known" energy levels are really known. There are misassignments, typos, mistakes, etc. Also, the Hamiltonians are approximate, so any lines that occur only because of mixing may not be very reliable. If laboratory measurements exist for such lines, the laboratory measurements are always preferable to the calculation. I collect all published data on gf values and include them in the line list whenever they appear to be more reliable than the current data.

I hope to spend the next year improving the line data. I will extend the atomic calculation to elements lighter and heavier than the iron group which I have already computed. Several of the iron group calculations have already been revised. I will recompute the energy levels and line lists whenever new laboratory analyses become available and I will make the predictions available to laboratory spectroscopists. Because computers are now more powerful, I will increase the number of configurations treated. This should account for more of the missing infrared lines because they are usually transitions between highly excited levels.

The new complication I have recently discovered (Kurucz 1992c) is that isotopic splitting is important in the iron group. Hyperfine splitting of the odd iron group elements is well known. It turns out that the even elements have significant isotope splitting. In general, all lines are asymmetric because of substructure when resolution and signal-to-noise are high enough. Velocity measurements from bisectors and Fourier profile analysis to determine microturbulent and macroturbulent velocities cannot be reliable. Isotopic splitting introduces systematic errors in abundances and wavelengths because weak components will still be on the linear part of the curve of growth when the stronger components are becoming saturated. These effects can be very strong in the infrared because even a small energy shift can be significant compared to the transition energy. There are practically no published measurements of isotope splitting for the iron group. However, if you go into James Brault's office and look through the piles of infrared spectra, splittings are clearly visible. Brault and Holweger (1981) have published data for a few lines of Ni I in the infrared where the four isotopes are resolved. The infrared Ti lines that are used for Zeeman studies have isotopic components, so those studies must have systematic errors. Analysis of Brault's spectra and new laboratory measurements are urgently needed.

At the present time I am including hyperfine and isotopic splitting one level at a time from whatever laboratory data I can find. Given enough laboratory data, I think it should be possible to work semi-empiricially to generate the splittings for my whole computed transition arrays. The unfortunate result will be 10 times as many lines. For molecules, the isotopic splitting is so large that it is always treated, but there is also hyperfine splitting that is normally ignored in stars.

My molecular data are all for diatomic molecules and are electronic transitions except for the CO vibration-rotation bands. Most of the calculations were done more than 15 years ago. I need to include all the improvements in the laboratory analyses since that time and I need to add all the significant vibration-rotation bands. The newer analyses are based on FTS spectra and produce dramatic improvements in energy levels and line positions. However, they still do not go to high enough V

and J. Farrenq *et al.* (1990) have actually been able to use the solar spectrum itself in the *ATMOS* atlas to analyse CO to high J.

I plan to distribute tapes and CD-ROMs with files of energy levels, damping constants, Landé g values, lifetimes, branching ratios, and line gf values. These should be useful to both laboratory and astronomical spectroscopists.

Acknowledgements

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