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REMAINING LINE OPACITY PROBLEMS FOR THE SOLAR SPECTRUM

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RESUMEN. Se necesita tener espectros solares de alta resolución y alta señal a ruido con cobertura espectral completa. El espectro solar provee la energía que controla la química atmosférica de la tierra y del resto de los cuerpos del sistema solar. Es importante para la astrofísica estelar porque constituye el espectro estelar "estándar", ya que puede ser observado mejor que el de cualquier otra estrella. Es importante para comprender al sol, ya que permite estudiar las condiciones y los movimientos en su superficie. Constituye un importante laboratorio de altas temperaturas para la espectroscopía atómica y molécular. Para interpretar este espectro se requiere tener conocimiento preciso sobre los niveles de energía, longitudes de onda, valores gf y constantes de amortiguamiento. Se requiere conocer los desdoblamientos hiperfino, isotópico y Zeeman. Se requiere completitud para deconvolucionar las confusiones de líneas espectrales. Se requiere conocer cada nivel que esté por debajo de la primera energía de ionización o disociación. Para las moléculas, esto significa conocer cada nivel vibracional y rotacional.

ABSTRACT. We need high-resolution, high-signal-to-noise spectra of the sun with complete spectral coverage. The solar spectrum provides the insolation that controls the atmospheric chemistry of the earth and of all the solar system bodies. It is important for stellar astrophysics as the "standard" stellar spectrum because it can be observed better than that of any other star. It is important for understanding the sun, for it allows us to study the conditions and motions at its surface. It is an important high-temperature laboratory source for atomic and molecular spectroscopy. To interpret the spectrum we require accurate energy levels, accurate wavelengths, accurate gf values, accurate damping constants. We require hyperfine splitting, isotopic splitting, and Zeeman splitting. We require completeness in order to deconvolve blends. We need every level below the lowest ionization or dissociation energy. For molecules that is every vibrational and rotational level.

Key words: ATOMIC PROCESSES - MOLECULAR PROCESSES - TRANSITION PROBABILITIES - SUN: SPECTRA

I. THE IMPORTANCE OF STUDYING THE SOLAR SPECTRUM

In the search for new results, the usual observational strategy of astronomers is to minimize signal-to-noise and resolution by observing objects as faint as possible. Whenever a new telescope or a better detector is built it is used to observe fainter objects instead of trying to understand the spectra of objects that can be well observed. The actual spectra consist 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 the best strategy is to study the brightest stars with the highest possible resolution and signal-to-noise. We can learn more about, say, globular clusters and the evolution of the galaxy by studying the brightest stars well, rather than by numerous poor observations. The sun is the brightest star available to us. It is possible to observe the solar spectrum with a signal-to-noise of 10000 and a resolving power of 1000000 at insignificant cost compared to most space projects. But nobody does. 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. In stars such lines might be much stronger and affect or dominate a crucial abundance determination, or some other investigation. The sun is also a good spectroscopic source for studying atoms and molecules. There are many cases where lines can be seen in the sun that have been difficult or impossible to see in the laboratory. Below I discuss the solar atlases that are available. There is very little available compared to what could be easily obtained, and there is very little compared to what is needed. The situation is disgraceful.

To be evenhanded, let me say that the laboratory situation is disgraceful as well. There is not one metal or molecule spectrum that I consider to be well analyzed. By that I mean that there are lines from that spectrum that appear in the sun or stars, and that matter in some way, but that are unidentified or unclassified. Half the lines in the solar spectrum are unidentified or unclassified. For relatively small amounts of money for modern spectrographs, lasers, and computers, one could make the analyses and even measure the oscillator strengths and damping constants along the way. People who work in this field barely receive support. I also know that this research historically has been very labor intensive, but computers are ideal for working with large masses of data, as I am sure I demonstrate below. Why is everyone afraid to be enthusiastic about basic science? Do everything, both in the laboratory and in theory. Then when we need data for our project of the moment, they will already be available.

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). All the stellar parameters can be varied to determine the most sensitive and easily measurable diagnostics. Then observing programs can be designed to measure those diagnostic features. The integrated spectra of clusters and galaxies can be treated in the same way. Below I discuss these computer projects and the line data.

II. 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. Figure 1 shows a small section of spectrum selected because it does not show dramatic discrepancies between the calculated and observed spectra.

III. 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 for the sun and the Griffins for the bright stars are committed to producing high-quality atlases. 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 every case the wavelength coverage is incomplete and higher quality is possible and needed. I have a review paper (Kurucz 1992) that shows each atlas plotted at very reduced scale. A sample is shown in Figure 2 to emphasize the complexity of a real spectrum.

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 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.

Observations made from ground-based observatories include the atmospheric transmission spectrum so 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 1000000 and a signal-to-noise greater than 10000. For atmospheric chemistry and planetary and cometary atmospheres, and for space-based stellar observations, however, the true flux spectrum above the atmosphere is required.

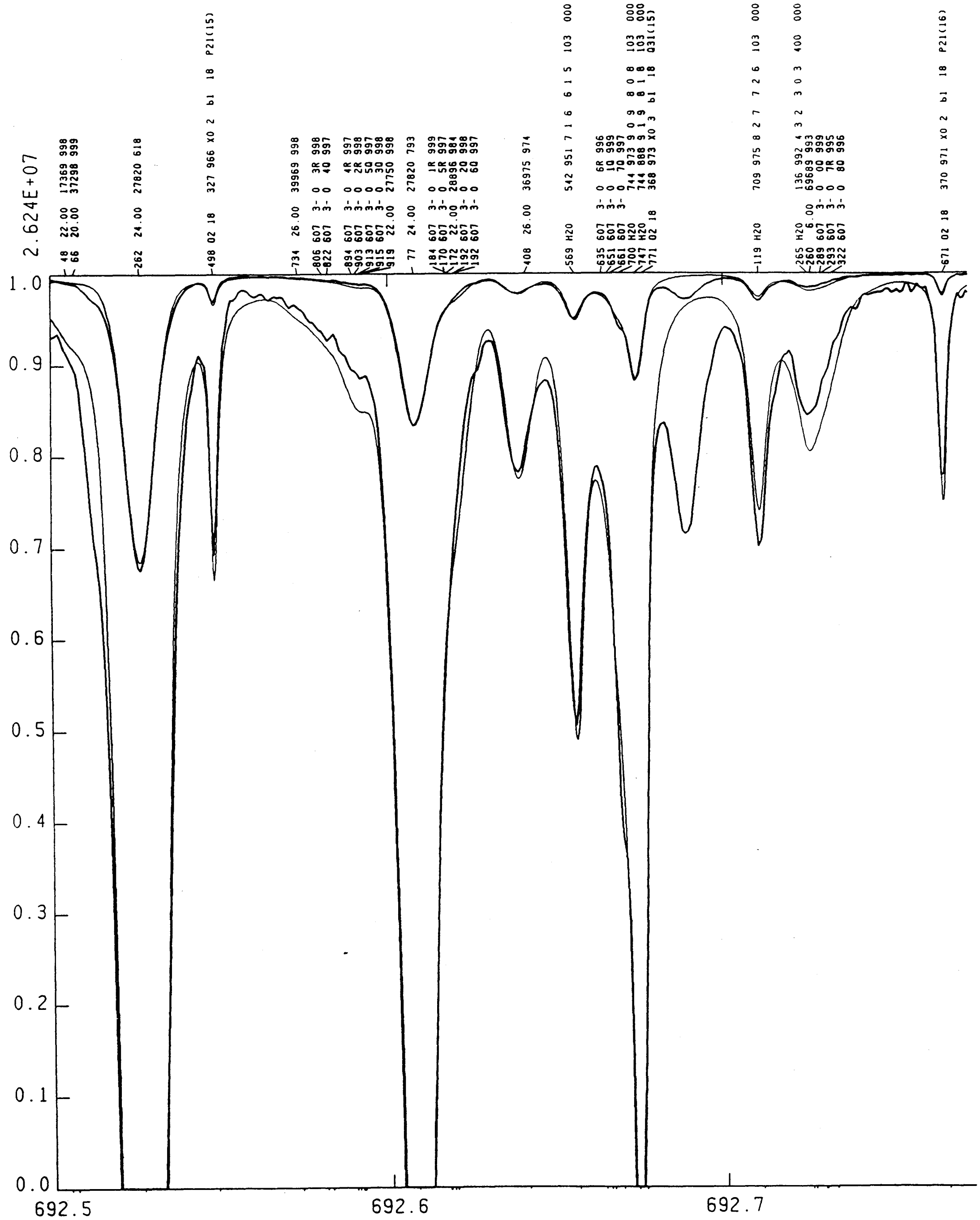

Figure 1 — A small section of solar central intensity spectrum at 692.5 nm plotted at full scale and at 10 times scale. The heavy lines are the observed FTS spectrum from James Brault at Kitt Peak. The resolution is 522000 and the signal-to-noise is about 3000 which is poor for this work. The continuum level is uncertain. The thin line is the computed spectrum. It would be possible to adjust the line data for a better match but most of the discrepencies are from missing lines. There are solar lines of Ca I, Ti I, Cr I, Fe I, C I, CN, and terrestrial lines of H_2O and $^{16}O^{18}O$. The first number in each line label is the last 3 digits of the wavelength and the 4th number is the per mil central intensity if the line were computed in isolation.

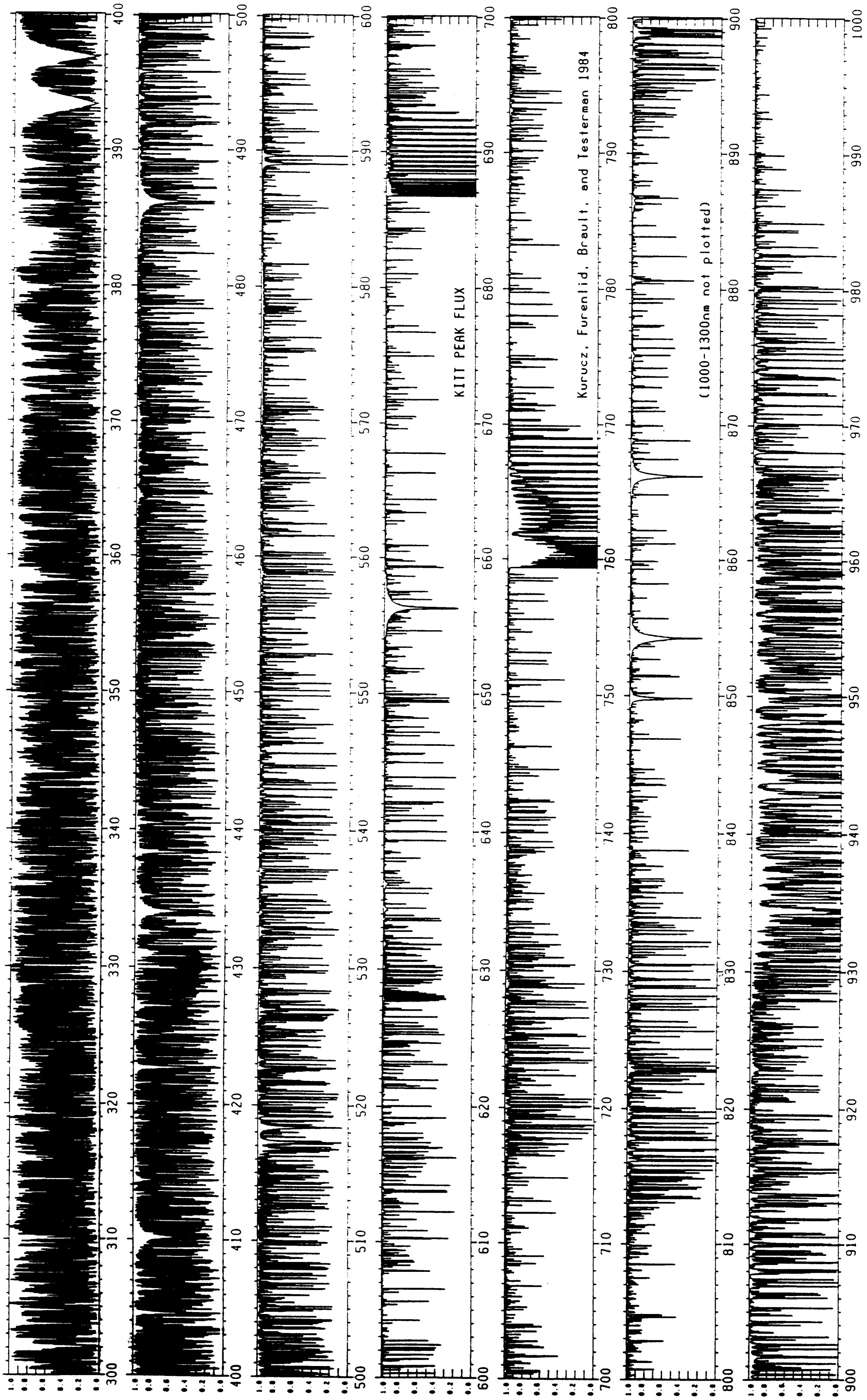

Figure 2 — The solar flux spectrum in the visible.

The solar flux atlas by Kurucz, Furenlid, Brault, and Testerman (1984) plots residual flux for 296 to 1300 nm 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. The resolving power is 522000 in the red and infrared and 348000 in the ultraviolet. The resolution is not high enough to resolve the terrestrial lines so there is some ringing. The atlas was fitted together from 8 overlapping scans that have reasonable signal-to-noise at the center but fall off in the region of overlap. In the final spectrum the signal-to-noise varies from 2000 to 9000. Ideally an atlas should be made from many more overlapping scans so that only near maximum regions need be used. The wavelength scale was set from a terrestrial O_2 line. The continuum level was estimated from high points and it is uncertain, especially in the ultraviolet. There are also problems caused by broad structures in the atmospheric transmission produced by ozone and O_2 "dimer".

The flux spectrum has been poorly observed. The existing atlas covers only the ground based spectrum in the visible. It is very high quality by astronomical standards but still leaves considerable room for improvement. There are no high-resolution flux atlases covering other wavelength regions or 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 semiempirical: 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. At present computing a realistic spectrum 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. Spectro-spectraheliograms 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 best central intensity spectrum in the visible is the Jungfraujoch atlas by Delbouille, Roland, and Neven (1973). The spectrum was observed in small wavelength sections from 300 to 1000 nm using a rapid-scanning double-pass monochrometer. The resolving power is greater than 350000 and the signal-to-noise is greater than 5000 by my guess. The wavelengths were set from Pierce and Breckinridge's (1973) line list. The wavelengths are not accurate in the 900 nm region because of lack of wavelength standards. I am reducing Brault's FTS spectra that will provide good wavelengths in this region.

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.

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. I have obtained the data tapes, reduced them, and set the continuum level. These spectra show beautiful vibration-rotation bands of CO and hydrides.

The central intensity spectra taken by the Ultraviolet Spectrometer and Polarimeter on the Solar Maximum Mission spacecraft (SMM/ UVSP) are the best in the ultraviolet but will not be ready for publication until some time in 1992. Richard Shine et al. at Lockheed have reduced the region from 129 to 177 nm. I am working on the region from 180 to 350 nm. The instrument failed before the spectrum was completely scanned so there is a gap between the two sections. The resolution and signal-to-noise are low by visible standards but are still much better than previous work in the ultraviolet. Better spectra are not likely to be produced this century.

I plan to publish or republish atlases for the sun and bright stars with the lines labelled, 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.

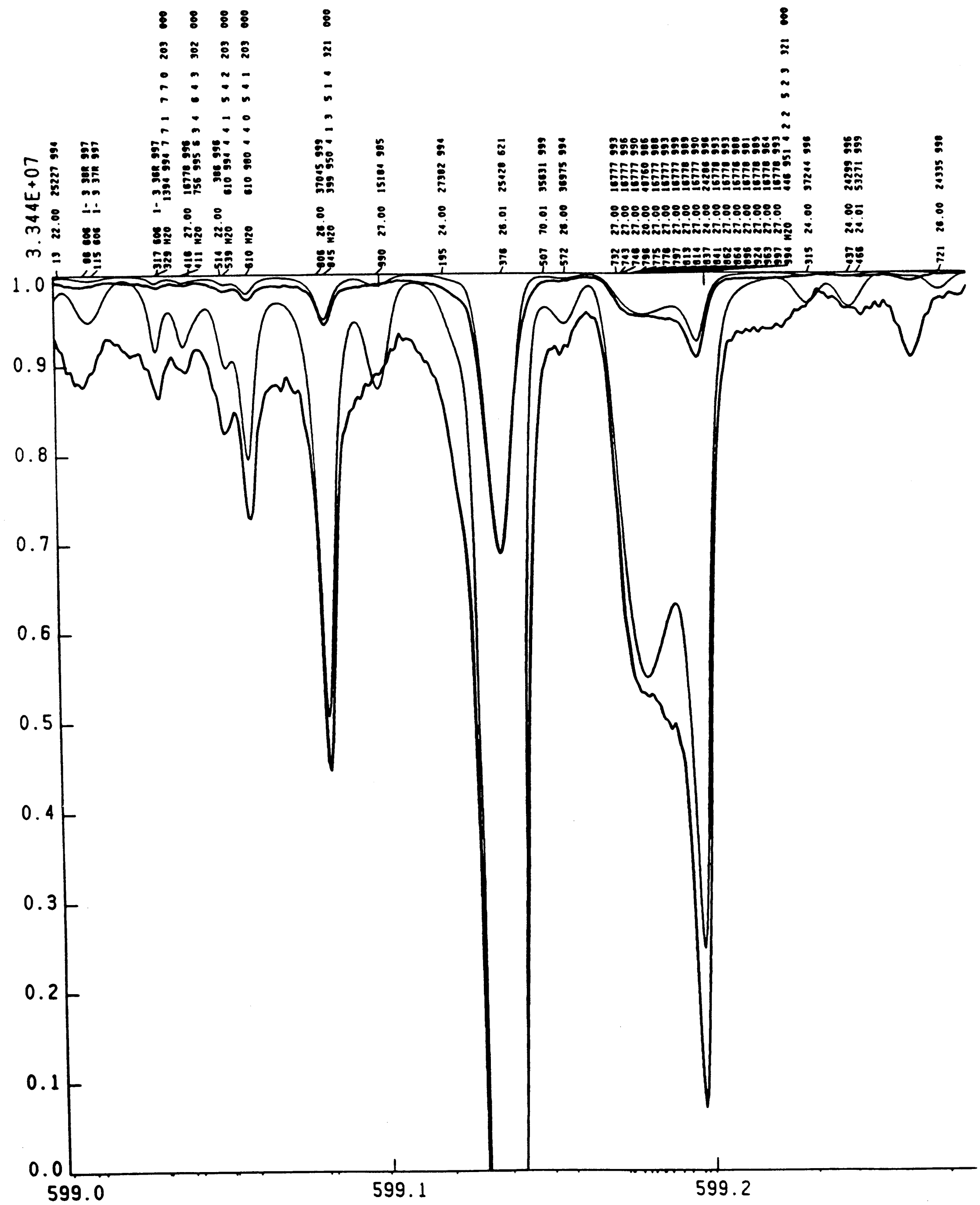

Figure 3 — A small section of solar central intensity spectrum at 599 nm plotted at full scale and at 10 times scale. The heavy lines are the observed FTS spectrum from James Brault at Kitt Peak. The resolution is 522000 and the signal-to-noise is about 3500 which is poor for this work. The continuum level is very uncertain due to atmospheric ozone. The thin lines are the computed spectrum. There are solar lines of Ca I, Ti I, Cr I, Cr II, Fe I, Fe II, Co I, Yb II, C_2, and terrestrial lines of H_2O. The first number in each line label is the last 3 digits of the wavelength and the 4th number is the per mil central intensity if the line were computed in isolation. The Co I line at 599.1866 has been divided into 15 hyperfine components. The hyperfine splitting is not known for the two other Co I lines. There are many missing lines.

IV. 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. I described my work on atomic and molecular line data in my first paper in this volume. Here I will mention only a few items.

When we talk about opacities for computing spectra we are in a completely different regime from that of statistical opacities. We require accurate energy levels, accurate wavelengths, accurate gf values, accurate damping constants. We require hyperfine splitting, isotopic splitting, and Zeeman splitting. We require completeness because we need to deconvolve blends. We need every level below the lowest ionization or dissociation energy. For molecules that is every vibrational and rotational level, not just the ones populated at low temperatures in the laboratory. Figure 3 shows examples of missing lines, blending problems, a Co I line with the hyperfine structure included, and Co I lines for which the hyperfine structure has not yet been determined.

There are weak atmospheric lines that are clearly present in our high-quality solar spectra but that are not yet in the HITRAN atmospheric line list (Rothman 1987). Better opacities for ozone and O_2 "dimer" are needed in the visible to determine the atmospheric transmission.

The simplest way to summarize is to say **more of everything, everything better,** and **everything computer readable**.

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