TSUJI: Your database is very extensive and can be used for many purposes from opacity calculation to high resolution spectral analysis. For these purposes, as the acuracy may be different for different lines, I wonder if you can give an indication of the accuracy of each line (e.g. by an additional code)?
KURUCZ: It would be possible to determine the sensitivity of the eigenvectors to small changes in the parameters and thus the sensitivity of the lines but I do not think it is worth the trouble. I never trust any of the calculations. There are uncertainties in the laboratory assignments. I can assign a level to the wrong eigenvalue. Either one of those mistakes ruins hundreds of lines. There are laboratory levels in the NBS books that do not exist. I believe in testing by comparing to very high resolution and very high signal-to-noise spectra.
GRIFFIN: You say that your models compute atmospheres for K giants, in which we know there is noticeable evidence for non-LTE. Are you able to estimate how your models compare with detailed empirical ones?
KURUCZ: No. I do know that my existing models are wrong because they do not include OH and SiO vibration-rotation bands. When I can get my opacity sampling model atmosphere program to converge properly, I will be check.

I have begun working with Fe I. Now there are many more levels known thanks to the efforts of Nave, Johansson, Learner, Thorne, and Brault 1994. Here is the result in numbers for electric dipole lines between observed levels,

	ultraviolet < 300 nm	< visible < 1000 nm	< infrared
1988	2140	9164	6839
1994	5919	17258	22167.

The new calculations will obviously have a large impact on spectrum analysis. I plan to double the size of my Hamiltonian matrices to include higher levels. That will produce a large increase in the number of predicted lines as well.

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DISCUSSION

COWLEY: A comment: For late-type stars, it doesn't matter how accurately the radiative transfer is done if the theory of convective transport is poor, and the theory of mechanical energy disposition into the upper layers is also poor. The models will still be uncertain.
KURUCZ: I agree, but remember that one also needs the opacities and radiative transfer to compute the convection correctly if it can ever be done.

C2DA.ASC	$^{12}C^{12}C$, $^{12}C^{13}C$, $^{13}C^{13}C$ Swan
C2EA.ASC	$^{12}C^{12}C$, $^{12}C^{13}C$, $^{13}C^{13}C$ Fox-Herzberg
CNAX.ASC	$^{12}C^{14}N$, $^{13}C^{14}N$, $^{12}C^{15}N$ Red
CNBX.ASC	$^{12}C^{14}N$, $^{13}C^{14}N$, $^{12}C^{15}N$ Violet
COAX.ASC	$^{12}C^{16}O$, $^{13}C^{16}O$, $^{12}C^{18}O$ 4th Positive
COXX.ASC	$^{12}C^{16}O$, $^{13}C^{16}O$, $^{12}C^{18}O$ vibration-rotation
H2.ASC	H_2 Lyman and Werner
HYDRIDES.ASC	^{12}CH, ^{13}CH A-X, B-X, C-X
	^{14}NH, ^{15}NH A-X, c-a
	^{16}OH, ^{18}OH A-X, X-X
	^{24}MgH, ^{25}MgH, ^{26}MgH A-X, B-X
	^{28}SiH, ^{29}SiH. ^{30}SiH A-X
SIOAX.ASC	$^{28}Si^{16}O$, $^{29}Si^{16}O$, $^{30}Si^{16}O$ $^{28}Si^{18}O$ A-X
SIOEX.ASC	$^{28}Si^{16}O$, $^{29}Si^{16}O$, $^{30}Si^{16}O$ $^{28}Si^{18}O$ E-X
SIOXX.ASC	$^{28}Si^{16}O$, $^{29}Si^{16}O$, $^{30}Si^{16}O$ $^{28}Si^{18}O$ vibration-rotation

CD-ROMs 20-22 provide the details of the iron group calculations that formerly were distributed on 28 magnetic tapes. Not many people will need these, but the information is useful for generating model atoms for non-LTE calculations.

NEW CALCULATIONS

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. 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. Several of the iron group calculations have already been revised. Because computers are now more powerful, more configurations can be treated. This should account for more of the missing infrared lines because they are usually transitions between highly excited levels. I will also try to include as much hyperfine and isotopic splitting data as possible (Kurucz 1993).

Some of my existing lists for diatomic molecules are fifteen years old and do not reproduce line positions very well for high v and high J. Almost every molecule has been reanalyzed using high quality FTS data. I will redo everything including all the new data, and I will add additonal bands down to the Lyman limit and all the missing vibration-rotation bands. In some cases I will have to re-reduce older ultraviolet data using the higher quality infrared data for the ground state.

I am redoing my iron group line list using the latest laboratory data. I will also do all the other elements and I will publish CD-ROMs as I go. The CDs will contain 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. There will be electric dipole, magnetic dipole, and electric quadrupole line lists. The line lists will be presented in several forms, packed and expanded. Some will have branching ratios. Laboratory measurements of gf values and lifetimes will be included. I am putting in hyperfine splitting and isotopic splitting for all lines that have empirical data.

known energy levels, regardless of perturbations. Lines to predicted levels are as accurate as the least squares fitting procedure. Radiative damping constants are automatically produced for each line.

Line lists for the triatomic molecules are needed for work on cool M stars. My list contains no triatomics at present. I hope to obtain them from Jørgensen and Jensen (1993) and other groups.

KURUCZ CD-ROMs

All my old data from the 80s are now available from me on CD-ROMs:

No. 1 Atomic data for opacity calculations.
No. 15 Diatomic molecular data for opacity calculations.
No. 18 SYNTHE spectrum synthesis programs and line data.
No. 20 Atomic Data for Ca, Sc, Ti, V, and Cr.
No. 21 Atomic Data for Mn and Co.
No. 22 Atomic Data for Fe and Ni.

CD-ROMs 1 and 15 contain all of my line data, 58 million lines, packed 16 bytes per line. The data packed are the minimum needed to compute a line profile: wavelength, identification, gf, lower energy level, radiative, Stark, and van der Waals damping constants. I use them to compute opacity-sampled model atmospheres, to compute complete spectra, and to tabulate Rosseland and wavelength dependent opacities. Programs for making such calculations will be distributed on CD-ROMs during the coming year.

CD-ROM 18 contains my spectrum synthesis programs, atomic line data files with lines between known energy levels with the spectroscopic detail included:
BELLHEAVY.DAT data collected from the literature by Barbara Bell for elements heavier than Ni
BELLLIGHT.DAT data collected from the literature by Barbara Bell for elements lighter than Ca if not already included in NLTELINES.DAT.
GFIRONLAB.DAT data collected from the literature for iron group elements
GULLIVER.DAT version of GFIRONLAB.DAT with data from Martin, Fuhr, and Wiese (1988) and Fuhr, Martin, and Wiese (1988) reformatted by Austin Gulliver.
NLTELINES.DAT (can be treated in non-LTE by Eugene Avrett) H I, He I, He II, B I, C I, C II, O I, Na I, Mg I, Mg II, Al I, Si I. Si II, K I, Ca I, Ca II . The ultraviolet series go to n=80 or 100 to merge with the continua.
GFIRONQ.DAT computed iron group line list described above.

The literature searches for the above files are not up to date. All these atomic line files will be merged into one file that will replace the old Kurucz-Peytremann (1975) line list. Having one file will simplify searching and sorting. It will be distributed as a CD-ROM.

Molecular line data files on CD-ROM 18:
C2AX.ASC $^{12}C^{12}C$, $^{12}C^{13}C$, $^{13}C^{13}C$ Phillips
C2BA.ASC $^{12}C^{12}C$, $^{12}C^{13}C$, $^{13}C^{13}C$ Ballick-Ramsay

data are available on CD-ROM 15 in packed form. All but the TiO are also on CD-ROM 18 in ASCII. The TiO is embarassingly low quality so that I refuse to give it out.

In 1983 I recomputed the opacities using the additional atomic and molecular data described above which totalled 17 million lines. These opacities were used to produce improved empirical solar models (Avrett, Kurucz, and Loeser 1984), but were found to still not have enough lines. In detailed ultraviolet spectrum calculations, half the intermediate strength and weak lines were missing. This discrepancy was caused by missing iron group atomic lines that go to excited configurations that had not yet been observed in the laboratory and so had not been included in the Kurucz-Peytremann calculations.

I was granted a large amount of computer time at the San Diego Supercomputer Center to carry out new calculations. I included as many configurations for each ion as I could fit into a Cray. Hamilitonian parameters were determined by combining least squares fits for levels that have been observed with computed Hartree-Fock integrals (scaled) for higher configurations. All configuration interactions were included. My computer programs 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 are automatically produced for each line. The first nine ions of Ca through Ni produced 42 million lines. Most of those lines have uncertain wavelengths because they go to predicted rather than measured levels. Only one per cent of the lines have reliable wavelengths because they connect laboratory determined energy levels. All the lines are on CD-ROM 1. The lines with reliable wavelengths are on CD-ROM 18. The computational details, least squares fits, etc., are on CD-ROMs 20-22.

Returning to the diatomic molecules, the line lists are in need of revision. All the transitions are electronic except for the CO, and recently added SiO and OH, vibration-rotation bands. Most of the isotopic positions are unreliable. Most of the calculations were done more than 15 years ago. I plan to include all the improvements in the laboratory analyses since that time, and I plan to add all the significant vibration-rotation bands and many ultraviolet electronic 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 to analyse CO to high J.

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 rotational Hamiltonian and then I do a least squares fit to determine the rotational constants. 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. 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. Since the known energy levels are used when available, the line wavelengths are correct for lines between

AN ATOMIC AND MOLECULAR DATA BANK FOR STELLAR SPECTROSCOPY

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ABSTRACT I am attempting to provide all of the basic atomic and diatomic molecular data needed to compute opacities, model atmospheres, and spectra. For opacity and model atmosphere calculations where only statistical accuracy is needed, the current list of 58 million lines, most with predicted wavelengths, works reasonably well. However, when computing spectra using only lines with good wavelengths, the quality is very poor. One half the lines are missing. Most of the gf values need to be corrected, and even the laboratory wavelengths are not always reliable. In addition, it now appears that hyperfine and isotopic splitting must be included because the quality of spectra is now high enough to show such effects.

All my old data are now available on CD-ROMs. I have now begun to recompute everything using the latest laboratory analyses. Next I will extend the calculations to all elements and to all significant diatomic molecules that now are missing from my list. I will also add as much hyperfine and isotopic data as possible. These new calculations will be distributed on CD-ROMs as they are produced.

OLD LINE DATA

My model calculations in the 1970s used the distribution-function line opacity computed by Kurucz (1979) from the line data of Kurucz and Peytremann (1975). We had computed gf values for 1.7 million atomic lines for sequences up through nickel using scaled-Thomas-Fermi-Dirac wavefunctions and eigenvectors determined from least squares Slater parameter fits to the observed energy levels. We also collected all published data on gf values and included them in the line list whenever they appeared to be more reliable than the computed data (that work is ongoing, but I am running behind).

After the Kurucz-Peytremann calculations were published, I started work on line lists for diatomic molecules beginning with H_2, CO, and SiO. Next, Lucio Rossi of the Istituto Astrofisica Spaziale in Frascati, John Dragon of Los Alamos, and I computed line lists for electronic transitions of CH, NH, OH, MgH, SiH, CN, C_2, and TiO. In addition to lines between known levels, these lists include lines whose wavelengths are predicted and are not good enough for detailed spectrum comparisons but are quite adequate for statistical opacities. All these