The Kurucz Smithsonian Atomic and Molecular Database

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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. 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 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.

1. 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 & Peytremann (1975).
We 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 H₂, 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, C₂, 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 data are available on CD-ROM 15 in packed form. All but
the TiO are also on CD-ROM 18 in ASCII. The TiO data is of such embarrassingly low quality that I refuse to give them 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 & Løesser 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, thus, 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. These calculations are described in Kurucz (1988). I included as many configurations for each ion as I could fit into a Cray. Hamiltonian 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 CO, and the 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 analyze 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 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 & Jensen (1993) and other groups.

2. The Kurucz CD-ROMs

All my old data from the 1980's 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 SYNTH 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 and atomic line data files with lines between known energy levels with the spectroscopic details 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 NLTE/LINES.DAT.
GFIRONLAB.DAT data collected from the literature for iron group elements.
NLT/LINES.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, and Ca II. The ultraviolet series go to n = 80 or 100 to merge with the continua.
The Kurucz Smithsonian Atomic and Molecular Database

GFIRONQ.DAT computed iron group line list as 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:

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2AX.ASC</td>
<td>$^{12}$C$^{12}$C, $^{12}$C$^{13}$C, $^{13}$C$^{13}$C Phillips</td>
</tr>
<tr>
<td>C2BA.ASC</td>
<td>$^{12}$C$^{12}$C, $^{12}$C$^{13}$C, $^{13}$C$^{13}$C Ballick-Ramsay</td>
</tr>
<tr>
<td>C2DA.ASC</td>
<td>$^{12}$C$^{12}$C, $^{12}$C$^{13}$C, $^{13}$C$^{13}$C Swan</td>
</tr>
<tr>
<td>C2EA.ASC</td>
<td>$^{12}$C$^{12}$C, $^{12}$C$^{13}$C, $^{13}$C$^{13}$C Fox-Herzberg</td>
</tr>
<tr>
<td>CNAX.ASC</td>
<td>$^{12}$C$^{14}$N, $^{13}$C$^{14}$N, $^{12}$C$^{15}$N Red</td>
</tr>
<tr>
<td>CNBX.ASC</td>
<td>$^{12}$C$^{14}$N, $^{13}$C$^{14}$N, $^{12}$C$^{15}$N Violet</td>
</tr>
<tr>
<td>COAX.ASC</td>
<td>$^{12}$C$^{16}$O, $^{13}$C$^{16}$O, $^{12}$C$^{18}$O 4th Positive</td>
</tr>
<tr>
<td>COXX.ASC</td>
<td>$^{12}$C$^{16}$O, $^{13}$C$^{16}$O, $^{12}$C$^{18}$O vibration-rotation</td>
</tr>
<tr>
<td>H2.ASC</td>
<td>H$_2$ Lyman and Werner</td>
</tr>
<tr>
<td>HYDRIDES.ASC</td>
<td>$^{12}$CH, $^{13}$CH A-X, B-X, C-X</td>
</tr>
<tr>
<td></td>
<td>$^{14}$NH, $^{15}$NH A-X, c-a</td>
</tr>
<tr>
<td></td>
<td>$^{16}$OH, $^{18}$OH A-X, X-X</td>
</tr>
<tr>
<td></td>
<td>$^{24}$MgH, $^{25}$MgH, $^{26}$MgH A-X, B-X</td>
</tr>
<tr>
<td></td>
<td>$^{28}$SiH, $^{29}$SiH, $^{30}$SiH A-X</td>
</tr>
<tr>
<td>SIOAX.ASC</td>
<td>$^{28}$Si$^{16}$O, $^{29}$Si$^{16}$O, $^{30}$Si$^{16}$O, $^{28}$Si$^{18}$O A-X</td>
</tr>
<tr>
<td>SIOEX.ASC</td>
<td>$^{28}$Si$^{16}$O, $^{29}$Si$^{16}$O, $^{30}$Si$^{16}$O, $^{28}$Si$^{18}$O E-X</td>
</tr>
<tr>
<td>SIOXX.ASC</td>
<td>$^{28}$Si$^{16}$O, $^{29}$Si$^{16}$O, $^{30}$Si$^{16}$O, $^{28}$Si$^{18}$O vibration-rotation</td>
</tr>
</tbody>
</table>

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.

3. 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 additional 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, C₄, C₆, and Landé g values. 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.

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

<table>
<thead>
<tr>
<th>Year</th>
<th>Ultraviolet &lt; 300 nm</th>
<th>Visible &lt; 1000 nm</th>
<th>Infrared</th>
</tr>
</thead>
<tbody>
<tr>
<td>1988</td>
<td>2140</td>
<td>9164</td>
<td>6839</td>
</tr>
<tr>
<td>1994</td>
<td>5919</td>
<td>17258</td>
<td>22167</td>
</tr>
</tbody>
</table>

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.

Acknowledgments

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References

The Kurucz Smithsonian Atomic and Molecular Database


Discussion

Jørgensen: The very limited comparison between OP and the CfA list indicate good agreement with a tendency of some of the CfA lines to be considerably weaker than the OP lines. Is any large-scale comparison planned? (This is a plea for such a comparison!)

Kurucz: They are not really comparable. I did detailed intermediate coupling calculations with all configuration interactions included. OP did LS coupling. Lines that appear only because of mixing do not even exist in the OP list, but appear in my list. Since the mixing is not computed perfectly, there is an intrinsic scatter that can be reduced only by improving the laboratory analysis.