Tables for stellar atmosphere opacity
Na broadened by He

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1 Summary

Each table "tableD_NaHe_T_1e21_GG.omg" contains coefficients for the expansion of the line profile opacity in density at a specific gas temperature.

They have been done for the D1 and D2 lines from T=150 to 2500 K for an He density = 10^{21} cm^{-3} and "tableD_NaHe_T_1e22_GG.omg" for an He density = 10^{22} cm^{-3} from T=3000 to 10000 K.

The "GG" is an annotation that these tables were computed using the *ab initio* potentials of Gregoire Guillon for the Na-He sytem. These potentials are described in Dell'Angelo et al (2012).

These new tables are valid up to a He density = 10^{21} cm^{-3} for T=150 to 2500 K, up to a He density = 10^{2} cm^{-3} from T=3000 to 10 000 K.

Previous Na-He tables were annoted "P83" as they were computed using the pseudo-potentials of Pascale (1983).

They were valid up to a He density = 10^{19} cm^{-3}.

They both use the density expansion described in Section 3.3 of Allard et al 2019.

The tables are consistently formatted and may be read by the Fortran or Python programs that are supplied with them.

2 Contents of the table files

Opacity for a grid of $\Delta\,\omega$ with frequency ω given in wavenumbers [cm^{-1}] relative to the unperturbed line center of the transition ω_0. That is, take the transition center in vacuum wavelength λ_0, find the line center in wavenumber

$$\overline{\nu}_0 = \omega_0 = 1/\lambda_0 \tag{1}$$

where $\overline{\nu}$ means "wavenumber", or frequency measured in units of cm^{-1}. and to that add the

$$\Delta\overline{\nu} = \Delta\omega \tag{2}$$

from the first column of the table to obtain the wavenumber for that opacity

$$\overline{\nu} = \omega = \overline{\nu}_0 + \Delta\overline{\nu} = \omega_0 + \Delta\omega \tag{3}$$

With that, compute the wavelength in vacuum

$$\lambda = 1/\overline{\nu} = 1/\omega \tag{4}$$

Note that the frequency "omega" implied by .omg filename and the notation ω is measured in wavenumber, that is in [cm^{-1}], *not* angular frequency in [radians/second]. Please see the comments below about setting the reference frequency from the reference atomic energy levels for the upper and lower states of the transitions.

3 Tables of expansion coefficients

These tables are formatted with space-delimited rows containing specific information for each $\Delta\omega$. They are annotated and must be read with a program that anticipates the format and the annotations.

The opacity table begins with a text header. The header is not needed to calculate opacity, but it contains information that may be useful in applications. The Python program provided parses a typical text header. The text header concludes with an "end" line.

The annotations are text before values. Most end with ":" but not all. These are text header entries and are not needed to parse the table.

Line numbers are relative to the first line starting with 1.

Line 1 – "Date of calculation: " followed by "day name month day-number hh:mm:ss year"

Line 2 – "TK: " followed by temperature floating point such as "1000.0"

Line 3 – "λ:" followed by reference line center in Å such as "5891.58"

The reference wavelength will be approximate, usually adequate for stellar spectra. For higher precision, consult the atomic energy level tables (AEL) for the relevant transitions. This would be important if the profiles are used in Phoenix where the transition line list has AEL precision.

Line 4 – "absorption oscillator strength fab" followed by floating point followed by cgs such as "0.64 cg". Note the absence of ":".

Line 5 – "r0 and fabs and pi*r0*fabs" followed by floating point such as "0.28000E-12 0.64080E+00 0.56368E-12". Note the leading space and absence of ":" Here "r0" is the classical radius of the electron, more precisely (than needed here)

$r_0 = 2.8179403227 \times 10^{-13}$ cm

and π r_0 f_{abs} is the area normalization constant for a line profile integrated over Δ ω.

Line 6 – "radiator perturber mass: " followed by two masses in AMU such as "23.00 4.0" for Na-He.

Note the leading space. These masses determine the atomic velocites and may be needed for other applications.

Line 7 – "perturber density [cm^{-3}]" followed by exponential format floating point such as "0.10000E+22"

Note the leading space, absence of ":". The contents of this line should match the file name density.

Line 8 –"omega cm^{-1}" followed by a text comment line including the order of the expansion.

A typical line is "$\Delta\omega$" in cm^{-1} from 1st order to the maximum order, and the maximum order is the number before "order". The maximum order depends on T.

Line 9 –"end" is self-explanatory and marks the end of the header block.

Following the text header there is a data header that must be read in order to calculate the opacities from the expansion coefficients. The Python and Fortran programs parse the data header.

Line 10 – Four floating point values, space delimited, needed to compute opacity. In order they are

- Line center wavelength in Å
- Reference perturber density for this table in cm^{-3}
- Normalization factor vn
- Normalization factor π r_0 f

Line 11 – Two integers, space delimited, need to compute the opacity.

- Number of table entries
- Maximum order of the expansion coefficient table

Line 12 – Two floating point numbers, space delimited, needed to compute the opacity (see Eq.14 of Allard et al 2019).

- Impact width in cm^{-1}
- Impact shift in cm^{-1}

The opacity table data blocks are 2 to 4 lines each, starting with line 13 and repeating in 2-line sets. The table ends on the last line of the last set, followed by a blank line. There are no other blank lines in the table. Thus we have at the beginning of the first data block

Line 13 – Series of floating point values, the first of which is $\Delta\omega$ in cm^{-1}.

Line 14 – A continuation of line 13 with more expansion coefficients.

Line 15 – A continuation of line 14 with more expansion coefficients.

Line 16 – A continuation of line 14 with more expansion coefficients.

The first entry of the set gives the frequency of that opacity. It is followed by 5 coefficients. The remaining lines have several coefficients each, but may be inconsistent from set to set. To read the table fully, a program must count the entries after the first one up to the number of terms in the expansion. The total should be the maximum order of the expansion (see Line 11), plus 1.

4 Programs

4.1 lect_sig.f

This Fortran program will read a"table" file and produce a"sigma" file. Use a script such as "lect_sig.sh" or "lect_sig.csh" to run this program with specific inputs.

First compile the program to produce an executable. On Linux, the compilation is done with

```
gfortran -o lect_sig lect_sig.f
```

to produce the executable "lect_sig" code. The program requires as input in order

densout – a flag that what follows is the density to use in computing the opacity

e-format float – the value of the density in cm^{-3}, for example 1.e21

domegc – a flag for frequency sampling for the core of the line

float – floating point value for the sampling, such as 0.5

nsf – a flag for the number of points calculated for the core

integer – integer count of the number of points to calculate in the core, such as 1000

text – the name of the table to use, such as tableD2_NaHe_T_1e21_GG.omg

4.2 lect_sig.sh or lect_sig.csh

The shell script will run under Bash (or the tcsh or csh shells). The extension is not needed, and would usually be".sh". Make the file executable under Linux this way

```
chmod a+x lect_sig.sh
```

If the file is in your PATH, then run it from the command line simply with its name. If it is not in your path, give the path to your current working directory (cwd). The file expects to find the table in the cwd, and will generate an opacity in that directory.

For example, use "ls" to find the files

```
ls
```

and you should see

```
lect_sig.sh
tableD2_NaHe_T_1e21_GG.omg
```

with the shell script and the table if that is to be the input. Then execute the script

```
./lect_sig.sh
```

and it will generate an opacity. Here the leading "./" runs the program in the cwd.

The contents of a typical script would be like this

```
#!/bin/sh

echo "Running lect_prof to generate opacities"
echo ""
lect_sig << %
densout
1.e21
domegc
0.5
nsf
1000
tableD2_NaHe_T_1e21_GG.omg
%
exit
```

where the first line is not needed on most systems. Note that the Fortran program executable "lect_sig" may need the"./" so that the system will find it. This depends on how the PATH of your system is set, so if in doubt, try

```
echo $PATH
```

to obtain a list of where your system will look for executable programs, in order.

The output will be four files

sigma_out.lam sigma_out.omg lorentz_out.lam lorentz_out.omg

that are respectively the wavelength-dependent opacity and the frequency-dependent opacity from this table, while lorentz_out.lam and lorentz_out.omg are the Lorentzian profiles for the core. The line parameters of these Lorentzian core files are the impact width and shift given in the tables.

4.3 alkali_opacity_from_expansion.py

This is Python 3 (tested under Python 3.7) program that has the same function as lect-sig. It requires input from the command line and does not need an auxiliary script (though you could use one). Make the program executable, and on a system where Python 3 is available simply run it with the command line arguments. The first line of the program assumes you will use your own local version of Python in "/usr/local/bin/" . Change this line if you are using Python in another location. On Windows, if you find it difficult to use the command line, modify the first part of the program to insert the values needed before running it.

The program is heavily commented and easily modified for other situations. The Python program will run with Anaconda Python if the first line is modified to point to its executable. If you use your system Python, set this to"/usr/bin/python3". On most Linux systems you may have to install additional packages to have the full set of Python modules you would get with Anaconda or building it yourself.

5 Tables of opacities

The tables (sigma_out.*, lorentz_out.*) are plain text files without internal comments or explanations, see D2/EXAMPLE_D2.

Data are space delimited in Unix file format with the first column the wavelength or frequency difference, and the second column the opacity.

These tables of opacity are derived from the expansion coefficients and are provided to be representative of the spectra that may be computed from the expansion coefficient tables with the programs provided (see lect_sig.csh, lect_sig.f, and alkali_opacity_from_expansion.py)

5.1 D2 component

See the example for the D2 component in D2/EXAMPLE_D2. Use lect5000_sig_test21.csh, lect_sig is run for a densout=1e21, for $T = 5000$ K with

```
#run lect\_prof
lect_sig <<
densout
1.e21
domegc
0.5
nsf
1000
../tableD2_NaHe_5000_1e22_GG.omg
%
exit
```

The obtained files are sigma_out.* and lorentz_out.*. The suffix "lam" is for wavelength in Å and"omg" is for relative frequency in cm^{-1}.
sigmaD2_NaHe21_T5000_lam.ps is a plot of sigma_out.lam and lorentz_out.lam
sigmaD2_NaHe21_T5000_omg.ps is a plot of sigma_out.omg and lorentz_out.omg.

These plot names contain the He density in cm^{-3} and the temperature in K.

The sampling for $\Delta\omega$ in the tables of expansion coefficients is not constant. It is very small close to the core to make easier the junction between the near wing and the core of the line given by the obtained Lorentzian profile lorentz_out.omg.

5.2 D1 component

See the example for the D1 component in D1/EXAMPLE_D1.

Compared to the tables provided in 2003, the new tables oversample the near wing to smoothly join the Lorentzian and the near wing.

sigmaD1_NaHe19_T1000_lam.ps and sigmaD1_NaHe19_T1000_omg.ps are the plots of the 2 parts which constitute the whole profile: the core given by the lorentz_out.*, the wing given by sigma_out.* .

5.3 JUNCTION and LOW DENSITIES

For the junction between the Lorentzian core and the wing the sampling "domegc" for the Lorentzian and "nsf" the number of points computed for the core have to be chosen as nsf $\times$ domegc to be larger than 3×10 cm^{-1}, 10 cm^{-1} being the sampling in the core.

The sampling "deomegc" and "nsf" have to be ajusted according to densout, i.e. for 10^{16} cm^{-3} to get the Lorentzian core, it requires 10000 points with deomegc = 0.005 cm^{-1} .

When dens_out gets very small, "domegc" decreases and "nsf" increases to provide the Lorentzian core accurately. The files will be large. Be careful of the dimension in the lect_sig.f program.