1. Download your transition line list from HITRAN

1. Go to the website hitran.org and register
2. Once your registration has been successful, go to the ‘Data Access’ tab and select ‘Line-by-line’
3. Select you desired molecule and make a note of the molecule number, then click on ‘2. Select isotopologues’
4. Make sure only the first isotopologue box is ticked, then make a note of the corresponding AFGL code (which we will need later) and click on ‘3. Select wavenumber / wavelength range’
5. Leave vmax as blank, and vmin as zero, and move on to ‘4. Select output options’
6. Click on ‘5. Start Data Search’
7. Download the .par file and save to your downloads folder (/home/*yourusername*/Downloads/)

2. Calculate absorption cross-sections

1. Open the command terminal. You should be in the directory /home/*yourusername*, which you can check by typing the command pwd (present working directory) into the command line. Move to your downloads directory by typing cd Downloads into the command line (where cd stands for change directory)
2. Now we need to find the partition function for your molecule. Type tipps.exe to run the tipps (total internal partition sum) executable and follow the prompts. When you are told to choose an isotopologue, type in the AFGL code you noted earlier. Select your desired temperature and make a note of the partition function *Q(T)*. Note: tipps will automatically return to step 1 after it’s displayed *Q(T)*, so press ctrl+c to exit the program.
3. Before we can calculate cross-sections we need to do one more thing. Making sure you’re still in your Downloads directory (/home/*yourusername*/Downloads), type the following into the command line: cp /home/prj/nercdtp/data/xcross\_input.inp ./ This copies the file xcross\_input.inp from the directory /home/prj/nercdtp/data/ to your current directory. Note: there is a space between cp and /home/ and another between .inp and ./
4. Type gedit sample\_input.inp into the command line to open the file sample\_input.inp with a text editor so that we can modify it
5. Modify the file as you wish but remember, your ‘iso’, ‘pf’ and ‘temperature’ input must match your selections thus far. Your ‘Transitions’ input should be the .par file that you downloaded in section 1. If you need to check the correct transitions file name close the text editor (ctrl+c in the command line) and type ls (list) into the command line to view all the files in your current directory.
6. Finally we can calculate the absorption cross-sections for your molecule at your chosen temperature by typing xcross.exe < xcross\_input.inp in the command line to launch the xcross executable with xcross\_input.inp as an input.

3. Plot your cross-sections

To plot your calculated cross-sections using the program xmgrace type xmgrace *your\_xcross\_output.*xsec and play around!

Useful Linux commands

cd /*full*/*path*/*to*/*directory* – change current directory to /*full*/*path*/*to*/*directory*

cd *directory* – move into the folder *directory* which is located in your current directory

cd .. – move to parent directory e.g move from /*full*/*path*/*to*/*directory* to /*full*/*path*/*to*

pwd – show present working directory

ls – list all files and directories in current directory

cp /*full*/*path*/*to*/*fileA* /*full*/*path*/*to*/*fileB* – copy *fileA* to *fileB*

cp *fileA* *fileB* – copy *fileA* in your current directory to *fileB* also in your current directory

more *file* – show contents of *file*