Peak-Picker Application for Excel

For the analysis if infrared spectra of DCl/HCl

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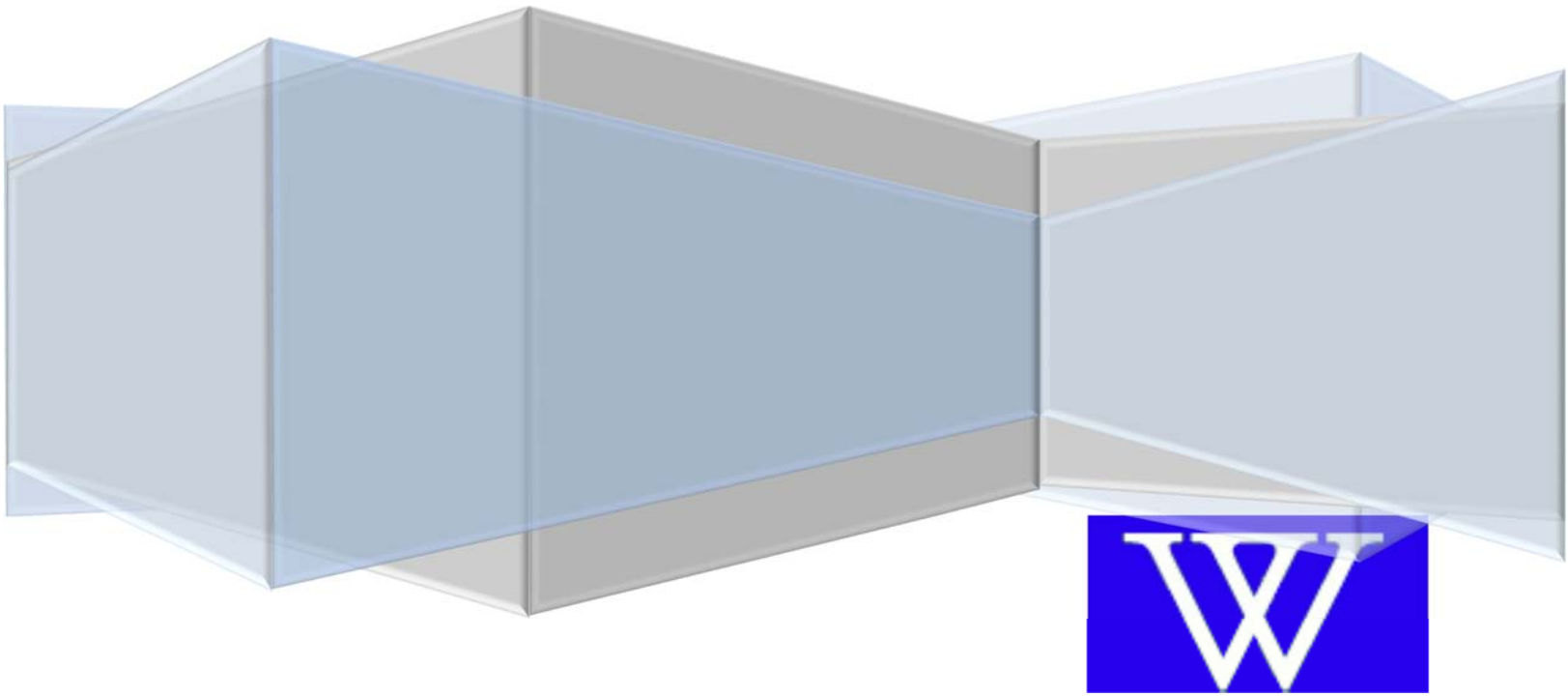
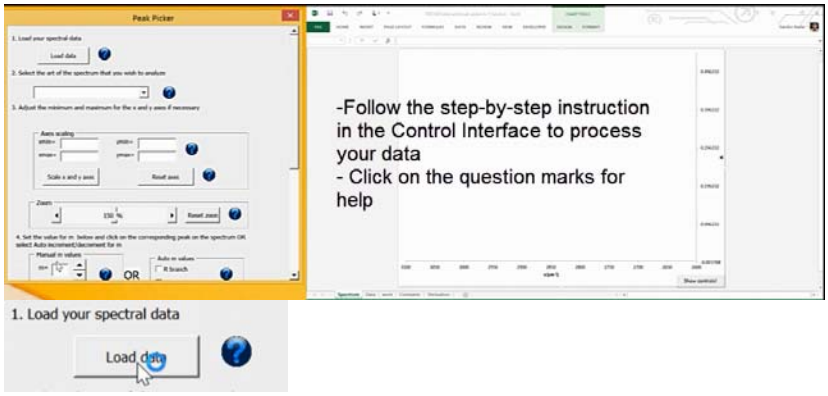


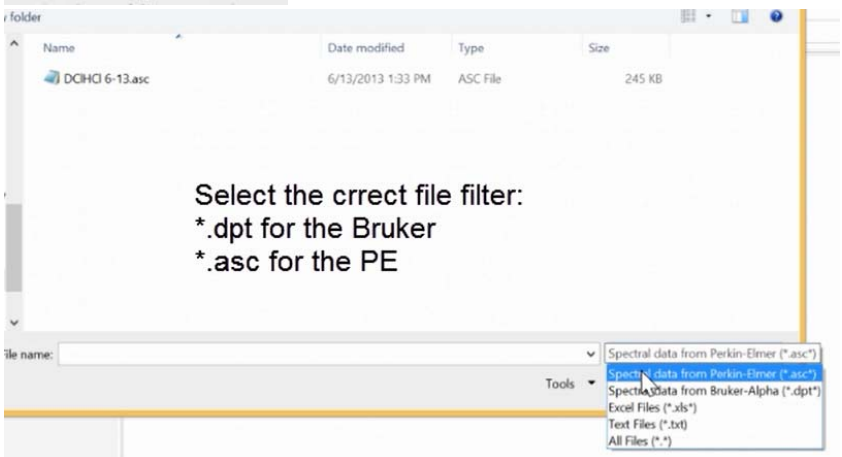
A spectrum can have 8 sections: one set of fundamental transitions for each of the four possible molecules ($D^{37}Cl$, $D^{35}Cl$, $H^{37}Cl$, $H^{35}Cl$), and the corresponding first overtones.

This application allows you to zoom in a section of the spectrum and collect the corresponding *m* and wavenumber data. You select the peaks by clicking on them and the program assigns the corresponding *m* value either automatically or you can do it manually. You analyze one set of transitions (e.g. $D^{37}Cl$ fundamental) at a time. Follow the steps in the form to collect data. The icons provide additional help

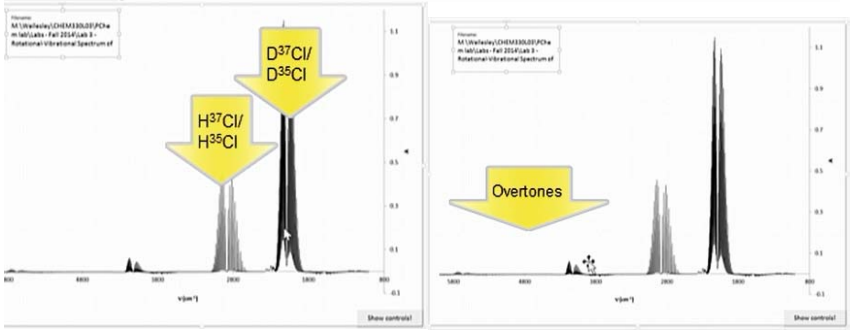
1. Open the application



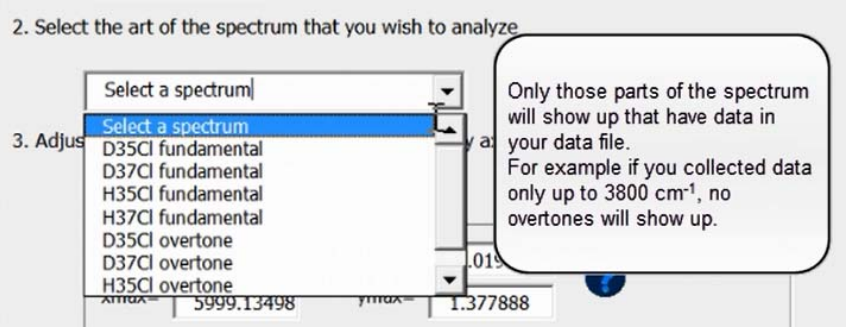
2. Click on the Load data button to load your data
3. Select the correct filter
   - For the PE instrument select "*.asc"
   - For the Bruker instrument select "*.dpt", and open your experimental file



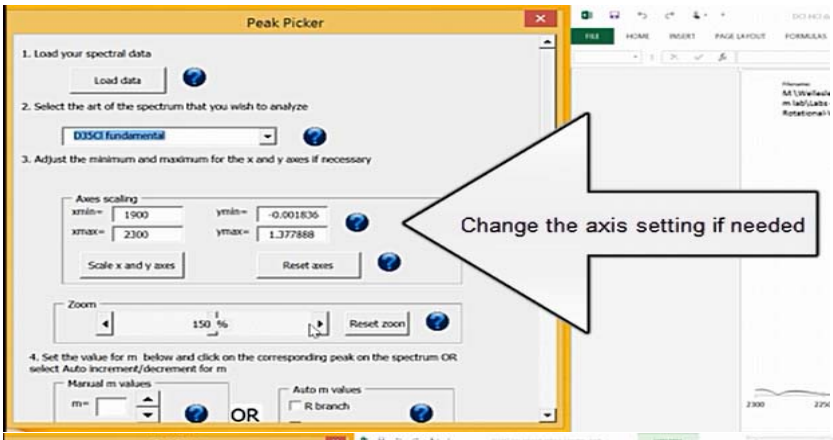
4. The spectrum will be displayed. Identify sections of the spectrum.



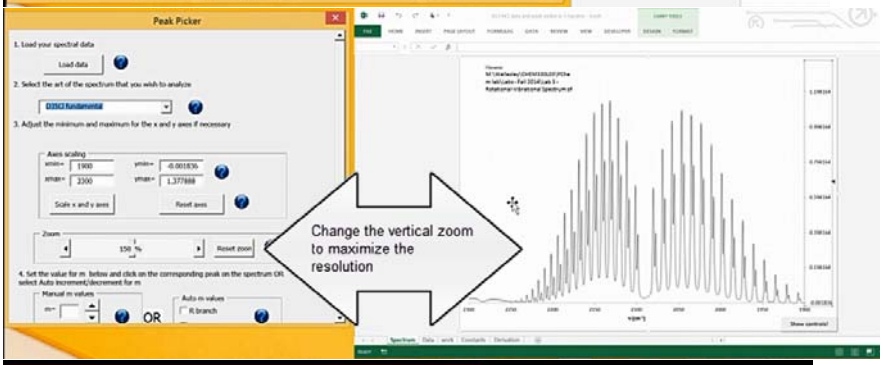
5. From the drop-down list select the a section of the spectrum to be analyzed (e.g. “D35Cl fundamental” for the n=0-> n=1 transition of the $D^{35}Cl$ molecule)
   - the selection will rescale the spectrum to show the part that you selected
   - only sections of the DCl/HCl spectrum will show up in the drop-down list for which the experimental data file has information for



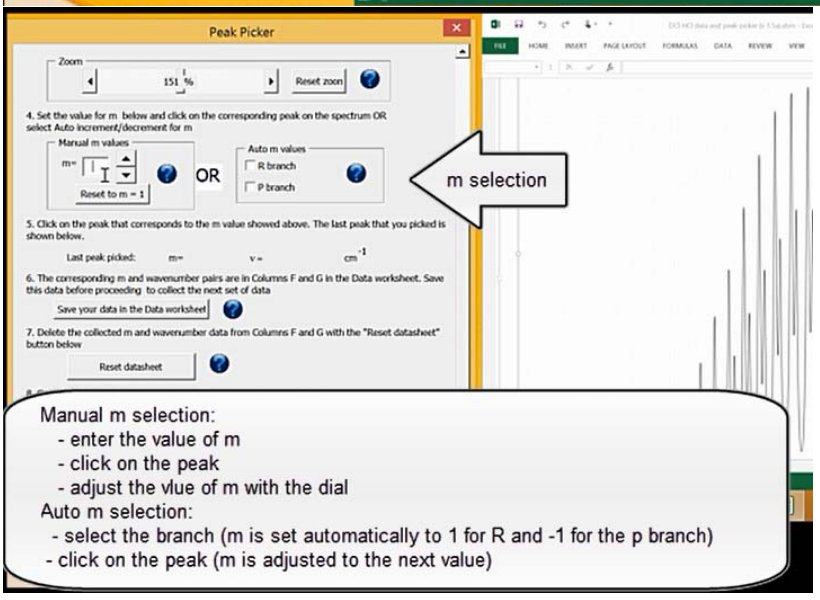
6. Adjust the scales if necessary by entering the new minimum and maximum values for the x and y axes and click on the Scale x and y axes button.
   - Click on the Reset axes button to show the whole spectrum again, if you need it



7. Adjust the vertical zoom to make the peaks that you analyze fill the graph



8. You can track the *m* values and the corresponding wavenumbers one of two ways: manually or automatically. For auto change of the *m* values:
   a. Check the Auto increment m option
   b. Then click on the peak which you think corresponds to *m* = 1. The value of *m* is incremented to *m* = 2.
   c. If the point is crrect, clickon OK, othwise click on NO and try again.
   d. Click on the peak *m* = 2.
   e. Continue until you are done with the R branch
   f. Select Auto decrement m (you need to click on it twice; the



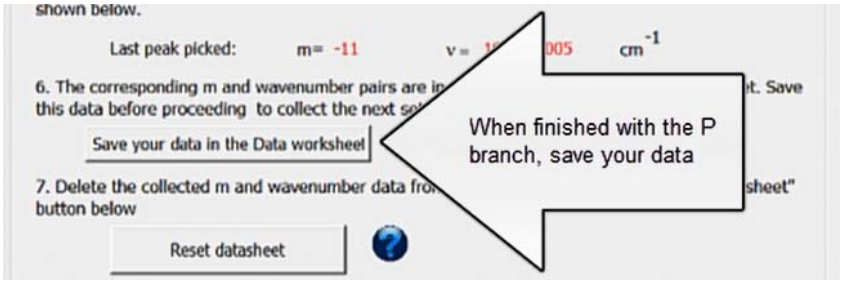
first click clears the auto-increment option)

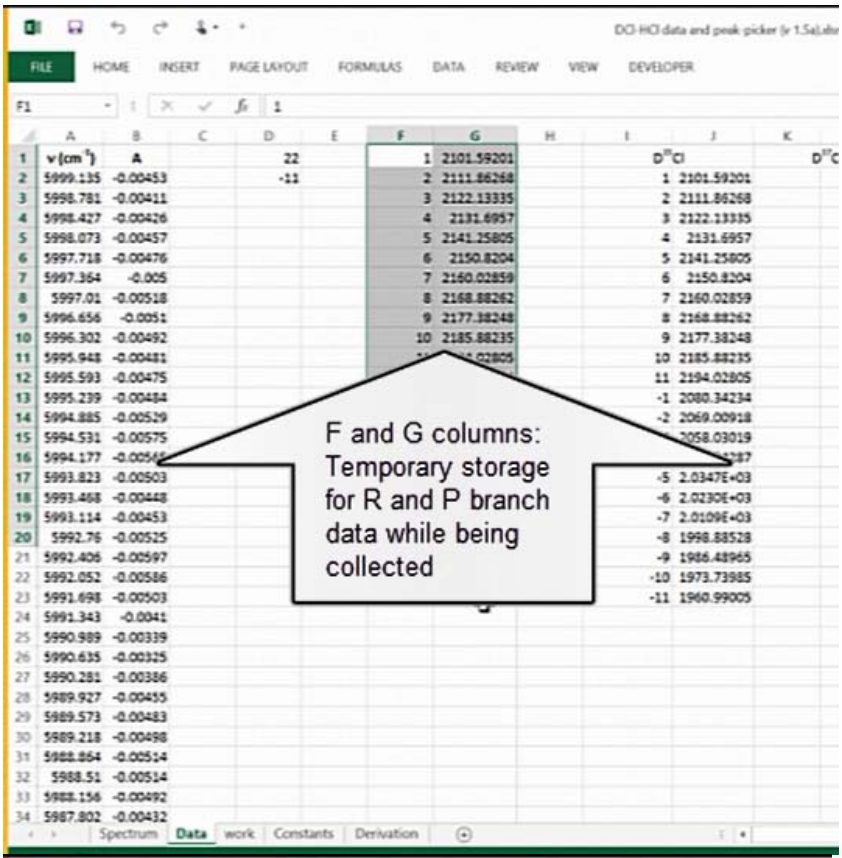
g. Then click on the peak which you think corresponds to *m* = -1. The value of *m* is decremented to *m* = -2.
h. Continue until you are done with the P branch

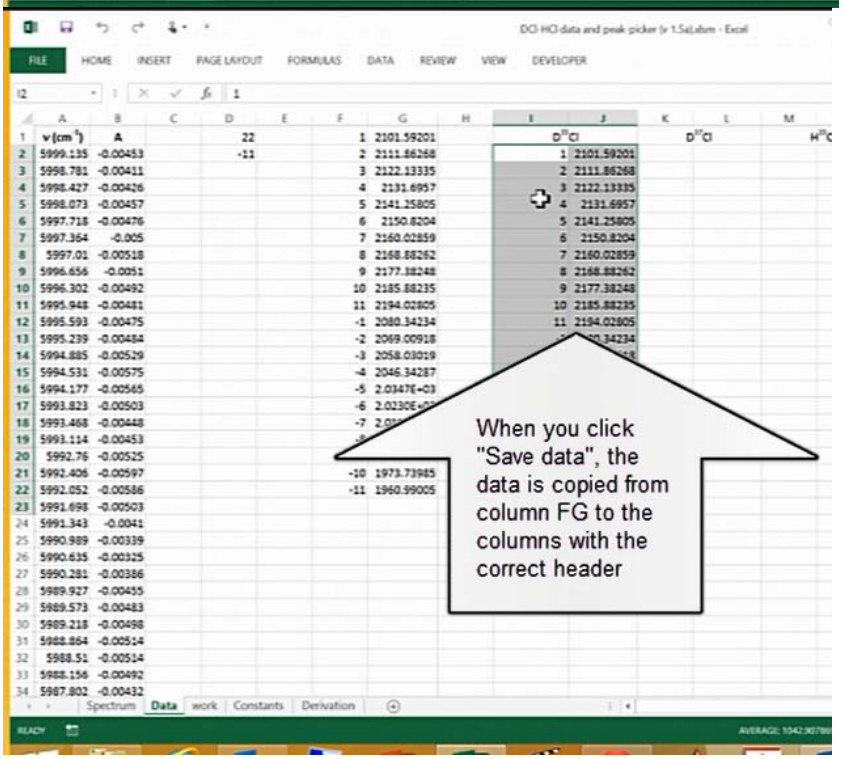
For manual adjustment of *m*, use the spin control:

a. Dial the *m* value
b. Click on the corresponding peak
c. Change the value of *m* by clicking up for the R branch
d. Continue until you collected all *m* values for the R branch
e. Click on the Reset to m = 0 button and once on the down arrow to set *m* = -1
f. Click on the first peak on the P branch
g. Keep changing the *m* value and clicking on the corresponding peak
   - If you make a mistake, just keep clicking until you get it right and then change *m*.

9. When you collected all the data, click on the Save your data in the Data worksheet button to save your data. This will save your data under the corresponding section in the "Data" worksheet and below the points in rows 35-39 shows the constants for a third-order polynomial fit.




F and G columns: Temporary storage for R and P branch data while being collected


When you click "Save data", the data is copied from column FG to the columns with the correct header

Below each set of data you can enter the formulae for the cubic polynomial fitting as shown in the figure. Note, that the function LINEST is used, for example:
=INDEX(LINEST(J2:J31,I2:I31^{1,2,3}), 1,2)
J2:J31 is the range of y values
I2:I31 is the range of x values
2 (at the end) refers to constant C
So this formula will calculates C (the quadratic term)