



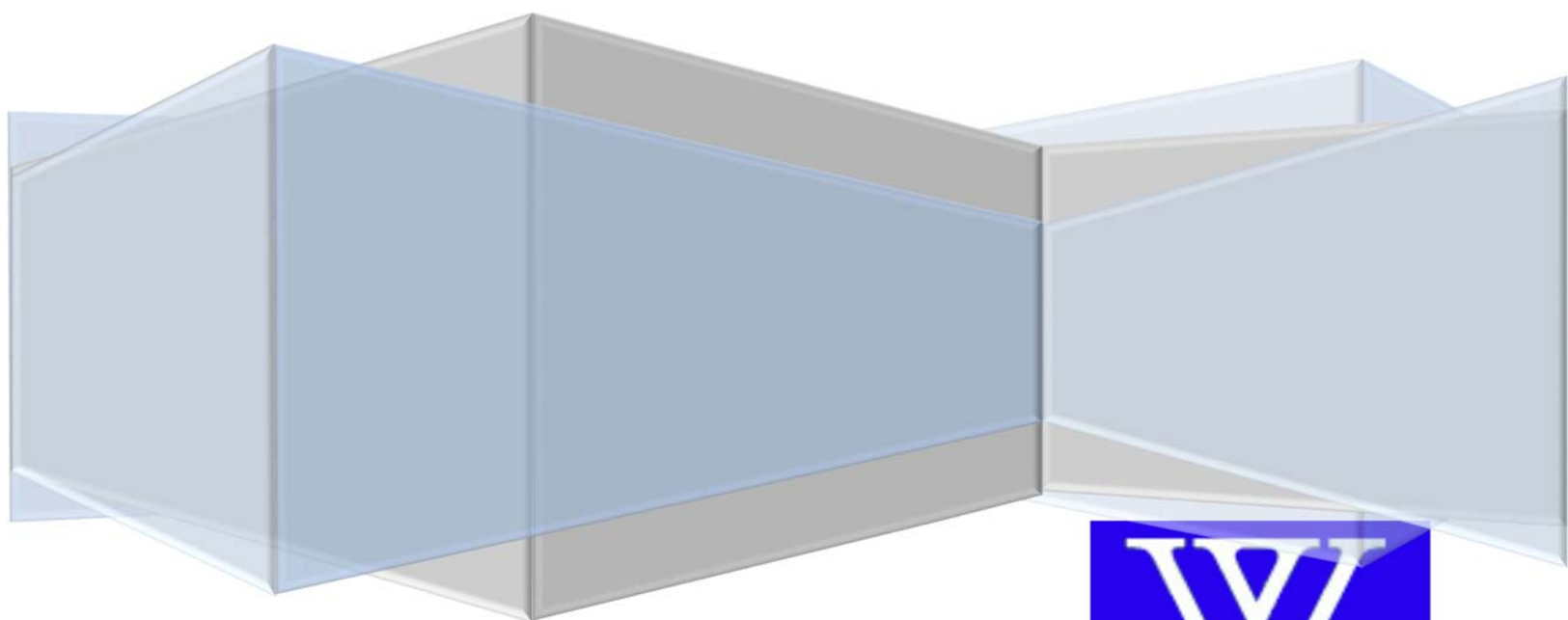
# Peak-Picker Application for Excel

For the analysis of 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.

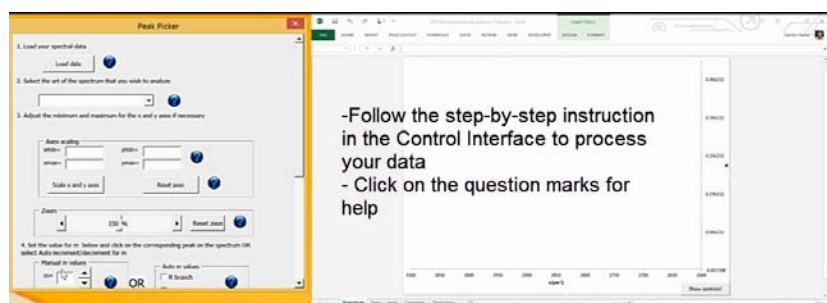
The video version of this manual is available from:

<http://chemistry4.me/PeakPicker.asp>

The program can be downloaded from:

[http://chemistry4.me/PeakPicker\\_app.asp](http://chemistry4.me/PeakPicker_app.asp)

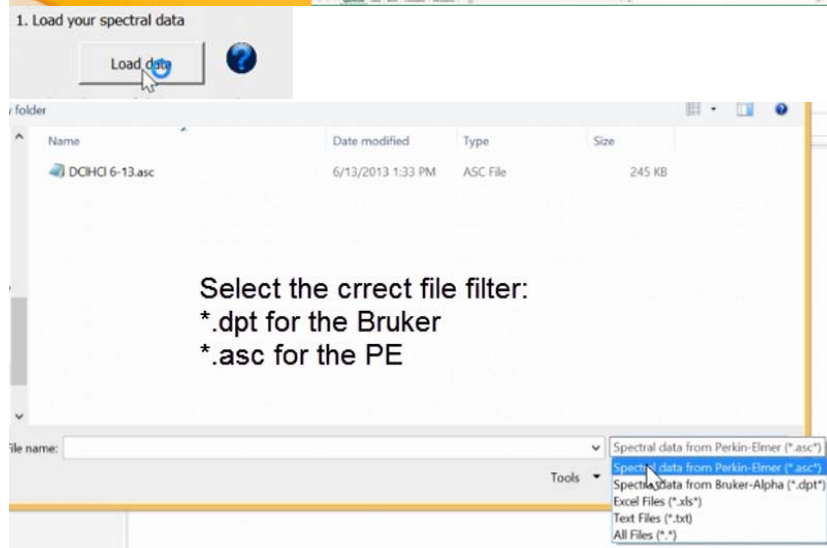
1. Open the application



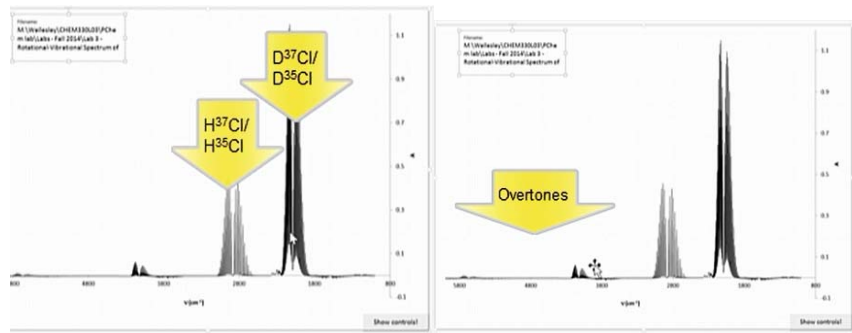
2. Click on the **Load data** button to load your data

3. Select the correct filter

- For the PE instrument select "\*.asc"
- For the Bruker instrument select "\*.dpt", and open your experimental file



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



- From the drop-down list select the a section of the spectrum to be analyzed (e.g. "D35Cl fundamental" for the  $n=0 \rightarrow n=1$  transition of the  $D^{35}Cl$  molecule)

- the selection will rescale the spectrum to show the part that you selected
- only sections of the DCI/HCl spectrum will show up in the drop-down list for which the experimental data file has information for

2. Select the part of the spectrum that you wish to analyze

3. Adjust

Select a spectrum

D35Cl fundamental  
D37Cl fundamental  
H35Cl fundamental  
H37Cl fundamental  
D35Cl overtone  
D37Cl overtone  
H35Cl overtone

Only those parts of the spectrum will show up that have data in your data file. For example if you collected data only up to  $3800\text{ cm}^{-1}$ , no overtones will show up.

- 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.

Scale x and y axes

- Click on the **Reset axes** button to show the whole spectrum again, if you need it

Reset axes

Peak Picker

1. Load your spectral data

Load data

2. Select the part of the spectrum that you wish to analyze

D35Cl fundamental

3. Adjust the minimum and maximum for the x and y axes if necessary

Axes scaling

xmin= 1900    ymin= -0.001836  
xmax= 2300    ymax= 1.377888

Scale x and y axes    Reset axes

Zoom 150 %    Reset zoom

4. Set the value for m below and click on the corresponding peak on the spectrum OR select Auto increment/decrement for m

Manual m values    OR    Auto m values

m=    R branch

Change the axis setting if needed

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

Peak Picker

1. Load your spectral data

Load data

2. Select the part of the spectrum that you wish to analyze

D35Cl fundamental

3. Adjust the minimum and maximum for the x and y axes if necessary

Axes scaling

xmin= 1900    ymin= -0.001836  
xmax= 2300    ymax= 1.377888

Scale x and y axes    Reset axes

Zoom 150 %    Reset zoom

4. Set the value for m below and click on the corresponding peak on the spectrum OR select Auto increment/decrement for m

Manual m values    OR    Auto m values

m=    R branch

Change the vertical zoom to maximize the resolution

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:

- Check the  Auto increment  $m$  option
- Then click on the peak which you think corresponds to  $m = 1$ . The value of  $m$  is incremented to  $m = 2$ .
- If the point is correct, click on OK, otherwise click on NO and try again.
- Click on the peak  $m = 2$ .
- Continue until you are done with the R branch

- Select  Auto decrement  $m$  (you need to click on it twice; the first click clears the auto-increment option)
- Then click on the peak which you think corresponds to  $m = -1$ . The value of  $m$  is decremented to  $m = -2$ .
- Continue until you are done with the P branch

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

- Dial the  $m$  value
- Click on the corresponding peak
- Change the value of  $m$  by clicking up for the R branch
- Continue until you collected all  $m$  values for the R branch
- Click on the  button and once on the down arrow to set  $m = -1$
- Click on the first peak on the P branch
- 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  $m$ .

4. Set the value for  $m$  below and click on the corresponding peak on the spectrum OR select Auto increment/decrement for  $m$

5. Click on the peak that corresponds to the  $m$  value shown above. The last peak that you picked is shown below.

Last peak picked:  $m =$   $v =$   $\text{cm}^{-1}$

6. The corresponding  $m$  and wavenumber pairs are in Columns F and G in the Data worksheet. Save this data before proceeding to collect the next set of data

7. Delete the collected  $m$  and wavenumber data from Columns F and G with the "Reset datasheet" button below

Manual  $m$  selection:  
 - enter the value of  $m$   
 - click on the peak  
 - adjust the value of  $m$  with the dial

Auto  $m$  selection:  
 - select the branch ( $m$  is set automatically to 1 for R and -1 for the p branch)  
 - click on the peak ( $m$  is adjusted to the next value)

Data point has a square around it  
If this data point is the peak, click OK

Last peak

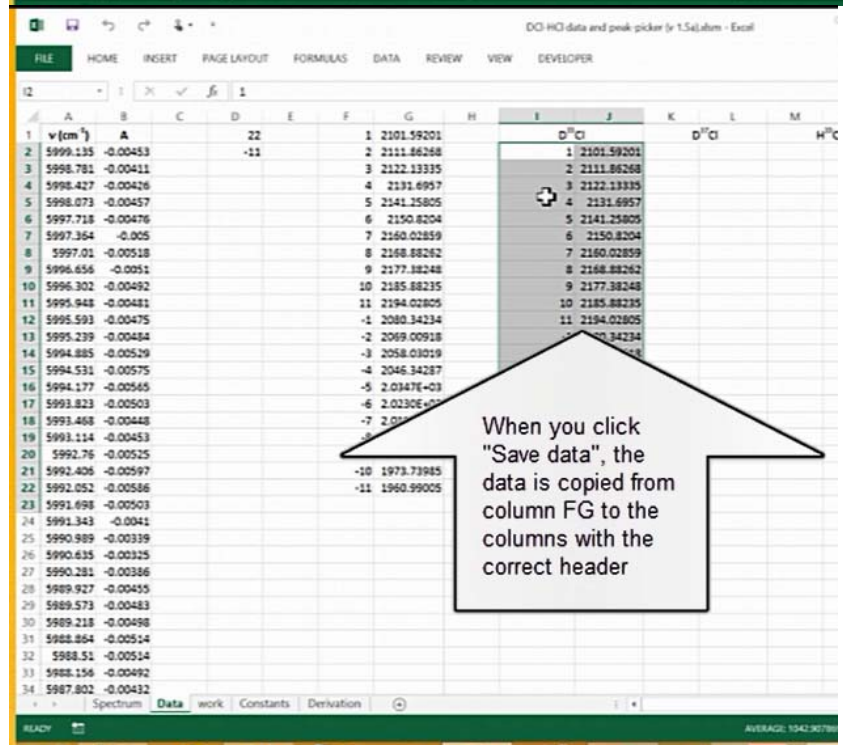
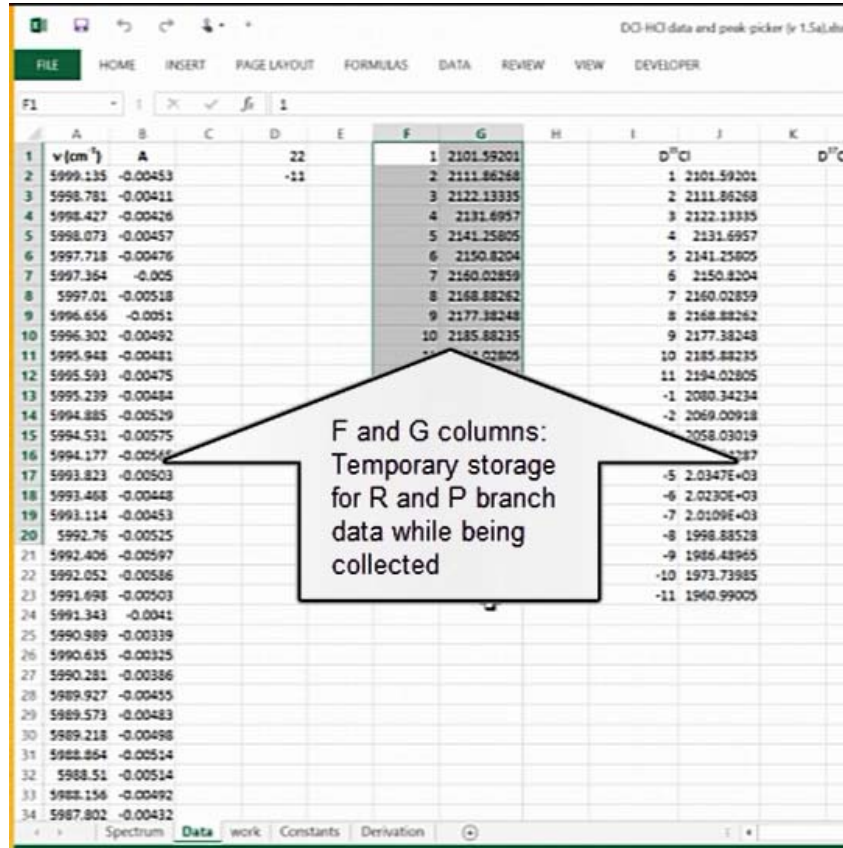
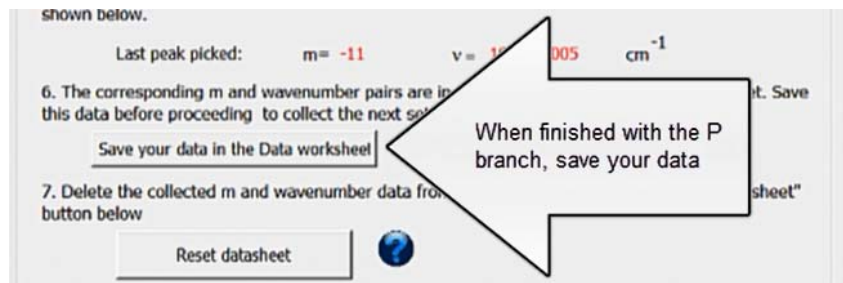
Keep this point?

Yes No

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.



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 calculate C (the quadratic term)

Data collected with peak p

INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER

$=INDEX(LINEST(J2:J31,I2:I31^{1,2,3}),1,4)$

	C	D	E	F	G	H	I	J
95							-13	1934.5
77							-14	1921
35							-15	1907.5
07								
31	$y(x) = A+Bx+Cx^2+Dx^3$ A: =INDEX(LINEST(J2:J31,I2:I31^{1,2,3}),1,4) B: =INDEX(LINEST(J2:J31,I2:I31^{1,2,3}),1,3) C: =INDEX(LINEST(J2:J31,I2:I31^{1,2,3}),1,2) D: =INDEX(LINEST(J2:J31,I2:I31^{1,2,3}),1,1)							
54								
13							D=	-0.0005452
24							C=	-0.1121755
44							B=	10.6693281
51							A=	2090.92317