



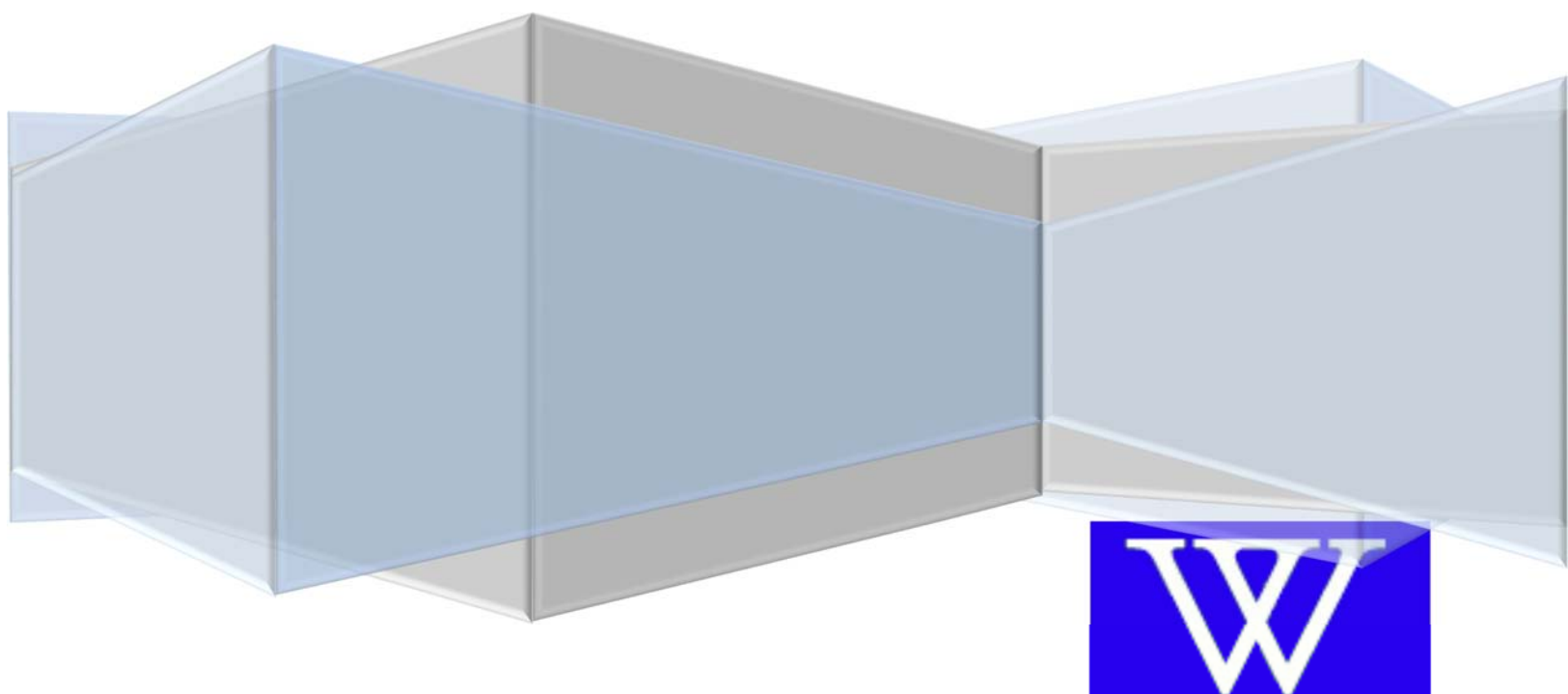
# Peak-Picker Application for Excel

For the analysis of infrared spectra of DCl/HCl

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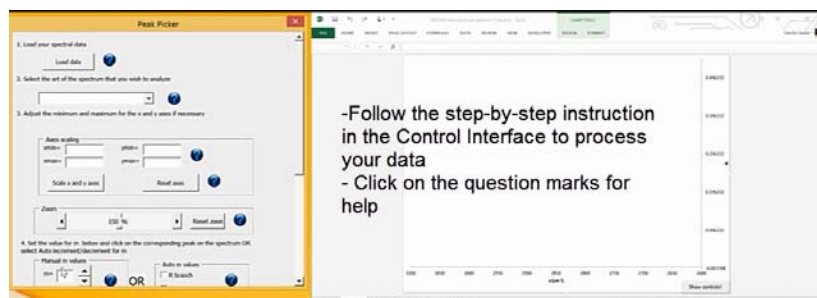


A spectrum can have 8 sections: one set of fundamental transitions for each of the four possible molecules ( $D^{37}Cl$ ,  $D^{35}Cl$ ,  $H^{37}Cl$ ,  $H^{35}Cl$ ), and the corresponding first overtones.

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



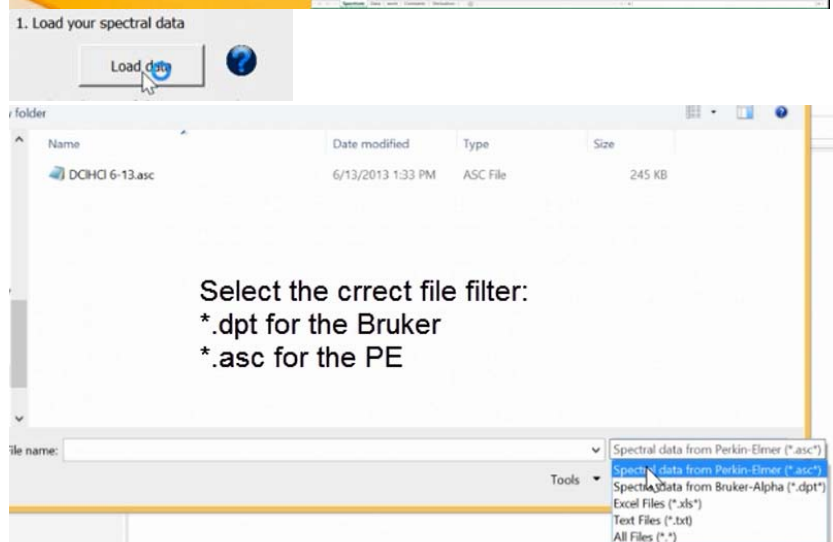
1. Open the application



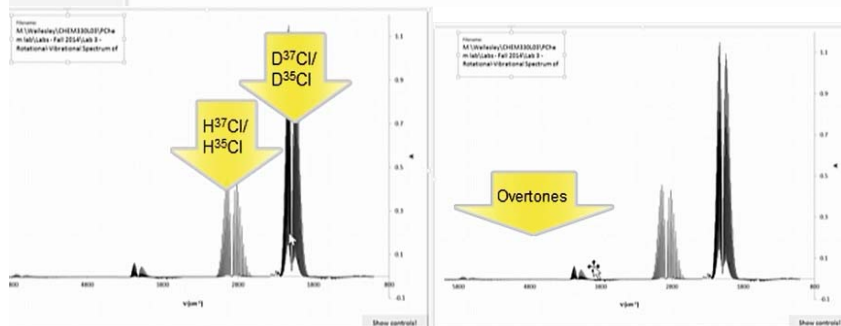
2. Click on the **Load data** button to load your data

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  $n=0 \rightarrow n=1$  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

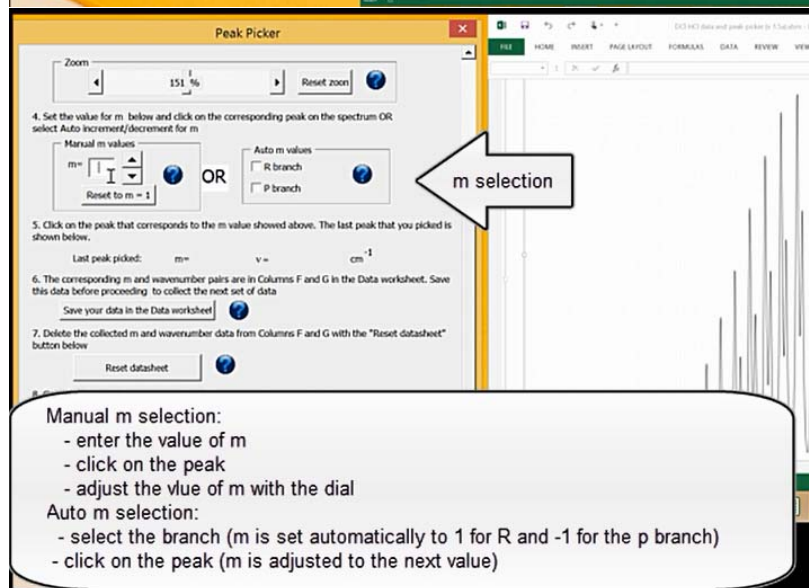
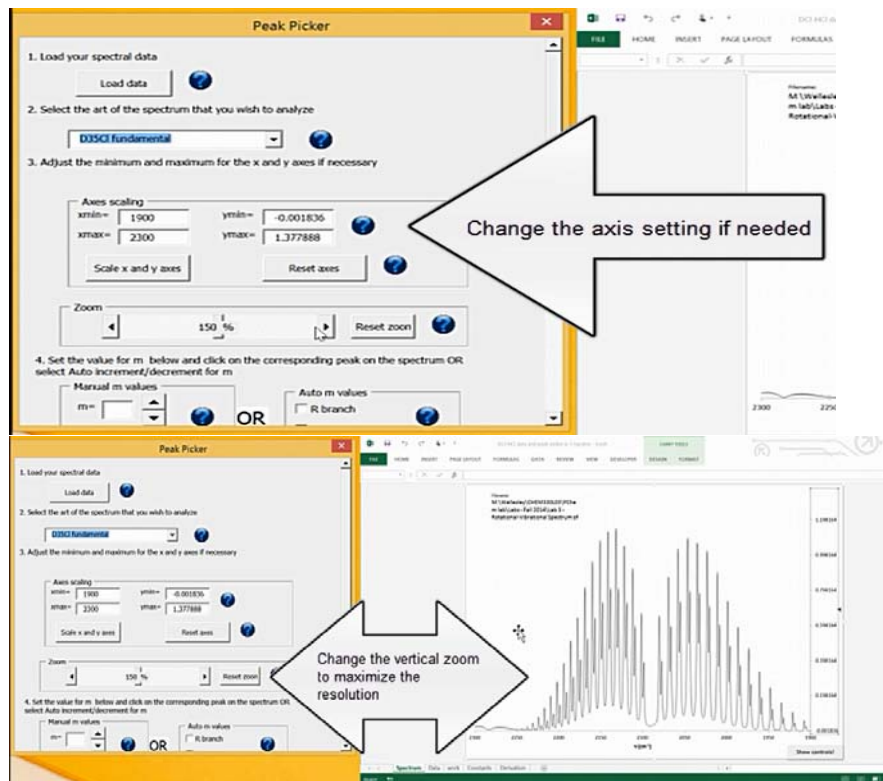
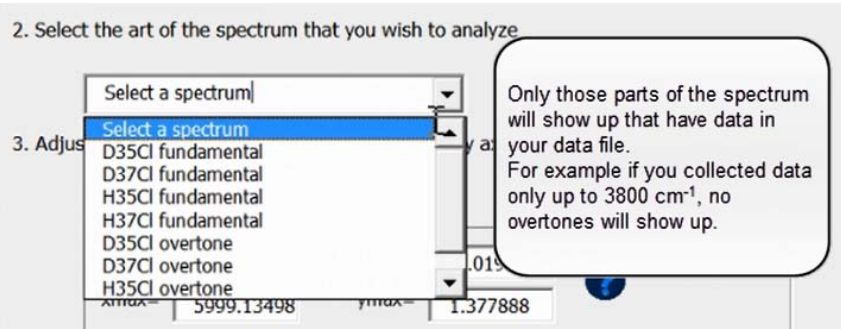
6. Adjust the scales if necessary by entering the new minimum and maximum values for the x and y axes and click on the **Scale x and y axes** button.

- 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:

- 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

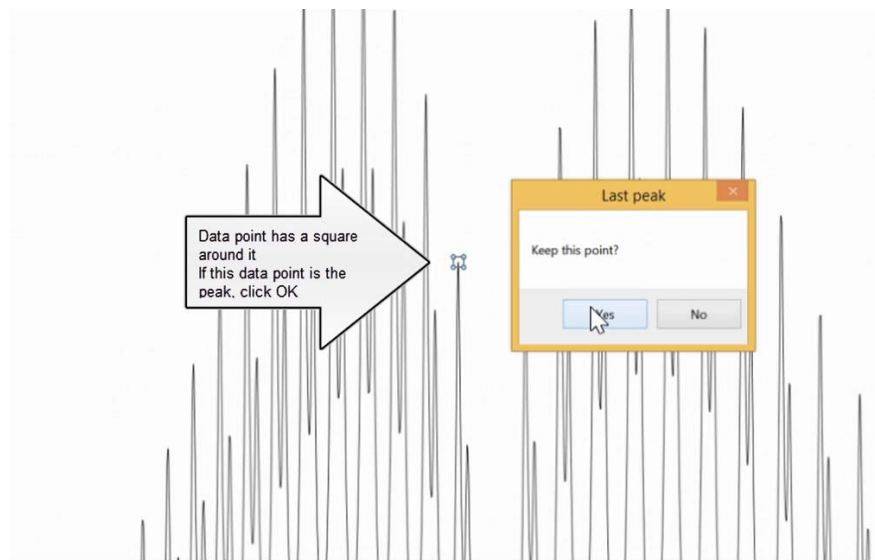


first click clears the auto-increment option)

- 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  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

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.

DO-HI data and peak picker (r 1.5a).xls

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER

F1

	A	B	C	D	E	F	G	H	I	J	K
1	v (cm <sup>-1</sup> )	A		22		1	2101.59201			D <sup>13</sup> C	D <sup>17</sup> C
2	5999.135	-0.00453		-11		2	2111.86268		1	2101.59201	
3	5998.781	-0.00411				3	2122.13335		2	2111.86268	
4	5998.427	-0.00426				4	2131.6957		3	2122.13335	
5	5998.073	-0.00457				5	2141.25805		4	2131.6957	
6	5997.718	-0.00476				6	2150.8204		5	2141.25805	
7	5997.364	-0.005				7	2160.02859		6	2150.8204	
8	5997.01	-0.00518				8	2168.88262		7	2160.02859	
9	5996.656	-0.0051				9	2177.38248		8	2168.88262	
10	5996.302	-0.00492				10	2185.88235		9	2177.38248	
11	5995.948	-0.00481				11	2194.02805		10	2185.88235	
12	5995.593	-0.00475				12	2202.34234		11	2194.02805	
13	5995.239	-0.00484				13	2209.00918		-1	2080.34234	
14	5994.885	-0.00529				14	2209.00918		-2	2069.00918	
15	5994.531	-0.00575				15	2205.83019		-3	2058.03019	
16	5994.177	-0.00565				16	2204.34287		-4	2046.34287	
17	5993.823	-0.00503				17	2203.067		-5	2.0347E+03	
18	5993.468	-0.00448				18	2202.30E+03		-6	2.0230E+03	
19	5993.114	-0.00453				19	2201.09E+03		-7	2.0109E+03	
20	5992.76	-0.00525				20	1998.88528		-8	1998.88528	
21	5992.406	-0.00597				21	1986.48965		-9	1986.48965	
22	5992.052	-0.00586				22	1973.73985		-10	1973.73985	
23	5991.698	-0.00503				23	1960.99005		-11	1960.99005	
24	5991.343	-0.0041									
25	5990.989	-0.00339									
26	5990.635	-0.00325									
27	5990.281	-0.00386									
28	5989.927	-0.00455									
29	5989.573	-0.00483									
30	5989.218	-0.00498									
31	5988.864	-0.00514									
32	5988.51	-0.00514									
33	5988.156	-0.00492									
34	5987.802	-0.00432									

Spectrum Data work Constants Derivation

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

DO-HI data and peak picker (r 1.5a).xls - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER

I2

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	v (cm <sup>-1</sup> )	A		22		1	2101.59201			D <sup>13</sup> C	D <sup>17</sup> C	H <sup>13</sup> C	
2	5999.135	-0.00453		-11		2	2111.86268		1	2101.59201			
3	5998.781	-0.00411				3	2122.13335		2	2111.86268			
4	5998.427	-0.00426				4	2131.6957		3	2122.13335			
5	5998.073	-0.00457				5	2141.25805		4	2131.6957			
6	5997.718	-0.00476				6	2150.8204		5	2141.25805			
7	5997.364	-0.005				7	2160.02859		6	2150.8204			
8	5997.01	-0.00518				8	2168.88262		7	2160.02859			
9	5996.656	-0.0051				9	2177.38248		8	2168.88262			
10	5996.302	-0.00492				10	2185.88235		9	2177.38248			
11	5995.948	-0.00481				11	2194.02805		10	2185.88235			
12	5995.593	-0.00475				12	2202.34234		11	2194.02805			
13	5995.239	-0.00484				13	2209.00918		-2	2069.00918			
14	5994.885	-0.00529				14	2209.00918		-3	2058.03019			
15	5994.531	-0.00575				15	2205.83019		-4	2046.34287			
16	5994.177	-0.00565				16	2204.34287		-5	2.0347E+03			
17	5993.823	-0.00503				17	2203.067		-6	2.0230E+03			
18	5993.468	-0.00448				18	2202.30E+03		-7	2.0109E+03			
19	5993.114	-0.00453				19	2201.09E+03		-8	1998.88528			
20	5992.76	-0.00525				20	1998.88528		-9	1986.48965			
21	5992.406	-0.00597				21	1986.48965		-10	1973.73985			
22	5992.052	-0.00586				22	1973.73985		-11	1960.99005			
23	5991.698	-0.00503				23	1960.99005						
24	5991.343	-0.0041											
25	5990.989	-0.00339											
26	5990.635	-0.00325											
27	5990.281	-0.00386											
28	5989.927	-0.00455											
29	5989.573	-0.00483											
30	5989.218	-0.00498											
31	5988.864	-0.00514											
32	5988.51	-0.00514											
33	5988.156	-0.00492											
34	5987.802	-0.00432											

Spectrum Data work Constants Derivation

READY AVERAGE: 1542.90788

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 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