

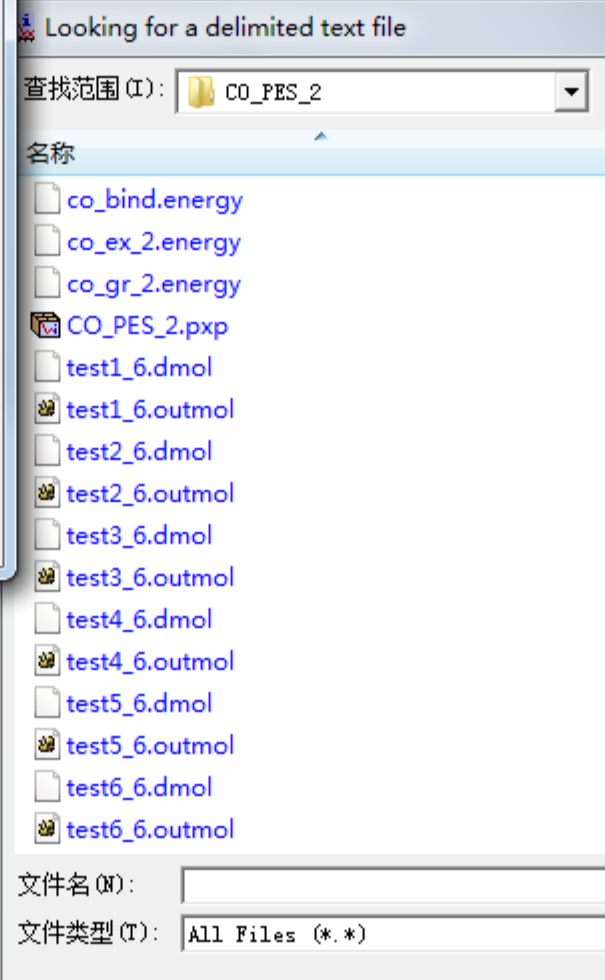
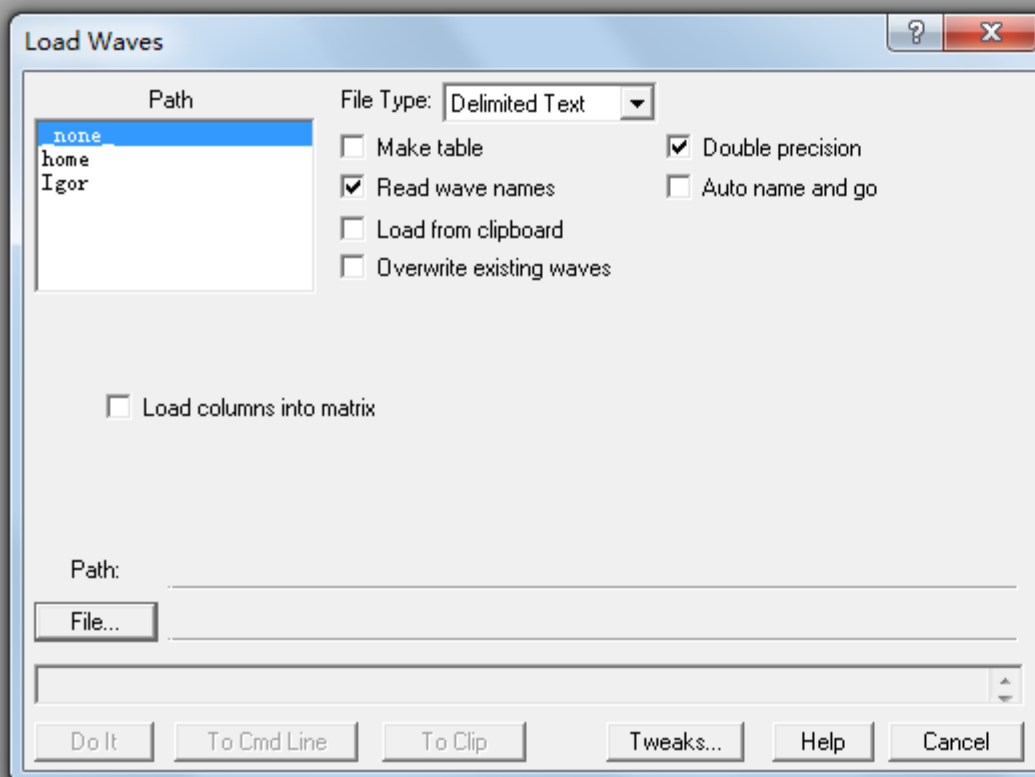
Loading data into Igor Standard method

Using the Data/Load Waves options

- Browse Waves...
- Load Waves ▶
- Save Waves ▶
- Make Waves...
- Duplicate Waves...
- Change Wave Scaling...
- Redimension Waves...
- Insert Points...
- Delete Points...
- Kill Waves...
- Rename...**
- Data Browser
- Packages ▶

Untitled

- Browse Waves...
- Load Waves ▶
 - Load Waves... Ctrl+L
 - Load Igor Binary...
 - Load Igor Text...
 - Load General Text...
 - Load Delimited Text...
 - Load Image...
 - Load General Binary File...
 - Load Excel File...
 - Packages ▶
- Save Waves ▶
- Make Waves...
- Duplicate Waves...
- Change Wave Scaling...
- Redimension Waves...
- Insert Points...
- Delete Points...
- Kill Waves...
- Rename...
- Data Browser
- Packages ▶



Loading data into Igor Useful Method

Cut and paste columns of data using
UltraEdit Column Mode



UltraEdit-32 - [C:\kazi\dft\CO\CO_PES_2\co_bind.energy]

File Edit Search Project View Format Column Macro Advanced Window Help

co_ex_2.energy | co_gr_2.energy | co_bind.energy

test2_6.outmol:df	-0.035558			14kcal/mol
test3_6.outmol:df	-0.151008			61kcal/mol
test4_6.outmol:df	-0.069975			11kcal/mol
test5_6.outmol:df	-0.139381			65kcal/mol
test6_6.outmol:df	-0.177741			37kcal/mol
test7_6.outmol:df	-0.228282			52kcal/mol
test8_6.outmol:df	-0.287587			67kcal/mol
test9_6.outmol:df	-0.350805			38kcal/mol
test10_6.outmol:df	-0.40894			622kcal/mol
test11_6.outmol:df	-0.43849			163kcal/mol
test12_6.outmol:df	-0.38332			542kcal/mol
test13_6.outmol:df	-0.11476			016kcal/mol
test14_6.outmol:df	0.66629			112kcal/mol
test15_6.outmol:df	2.66814			319kcal/mol
test16_6.outmol:df	7.4751982Ha	203.41058	4690.851kcal/mol	

- Column Mode Alt+C
- Insert/Fill Columns
- Delete Columns
- Cut Columns
- Insert Number
- Sum Columns/Selection
- Convert to Fixed Column
- Convert to Character Delimited
- Left Justify
- Center Justify
- Right Justify

Absorption
400 2

8000.0000	,0.11187107
8010.0000	,0.11696653
8020.0000	,0.12212091
8030.0000	,0.12732606
8040.0000	,0.13257391
8050.0000	,0.13785647
8060.0000	,0.14316598
8070.0000	,0.14849492
8080.0000	,0.15383608
8090.0000	,0.15918264
8100.0000	,0.16452822
8110.0000	,0.16986691
8120.0000	,0.17519333
8130.0000	,0.18050267
8140.0000	,0.18579073
8150.0000	,0.19105392
8160.0000	,0.19628929
8170.0000	,0.20149457
8180.0000	,0.20666814
8190.0000	,0.21180904
8200.0000	,0.21691699
8210.0000	,0.22199233
8220.0000	,0.22703607
8230.0000	,0.23204981
8240.0000	,0.23703573
8250.0000	,0.24199659
8260.0000	,0.24693568
8270.0000	,0.25185677
8280.0000	,0.25676411
8290.0000	,0.26166235

Table0:wave0

Point	wave0				
0	0.111871				
1	0.116967				
2	0.122121				
3	0.127326				
4	0.132574				
5	0.137856				
6	0.143166				
7	0.148495				
8	0.153836				
9	0.159183				
10	0.164528				

Untitled

```
rename wave0 absorb
```


Table0:wave0

Point	wave0
0	0.111871
1	0.116967
2	0.122121
3	0.127326
4	0.132574
5	0.137856
6	0.143166
7	0.148495
8	0.153836
9	0.159183
10	0.164528

Rename Objects

Waves

Current Name	Type	New Name
wave0	Wave	absorb

Rename wave0, absorb;

Do It To Cmd Line To Clip Help Cancel

Untitled

Ready

Table0:absorb,rr

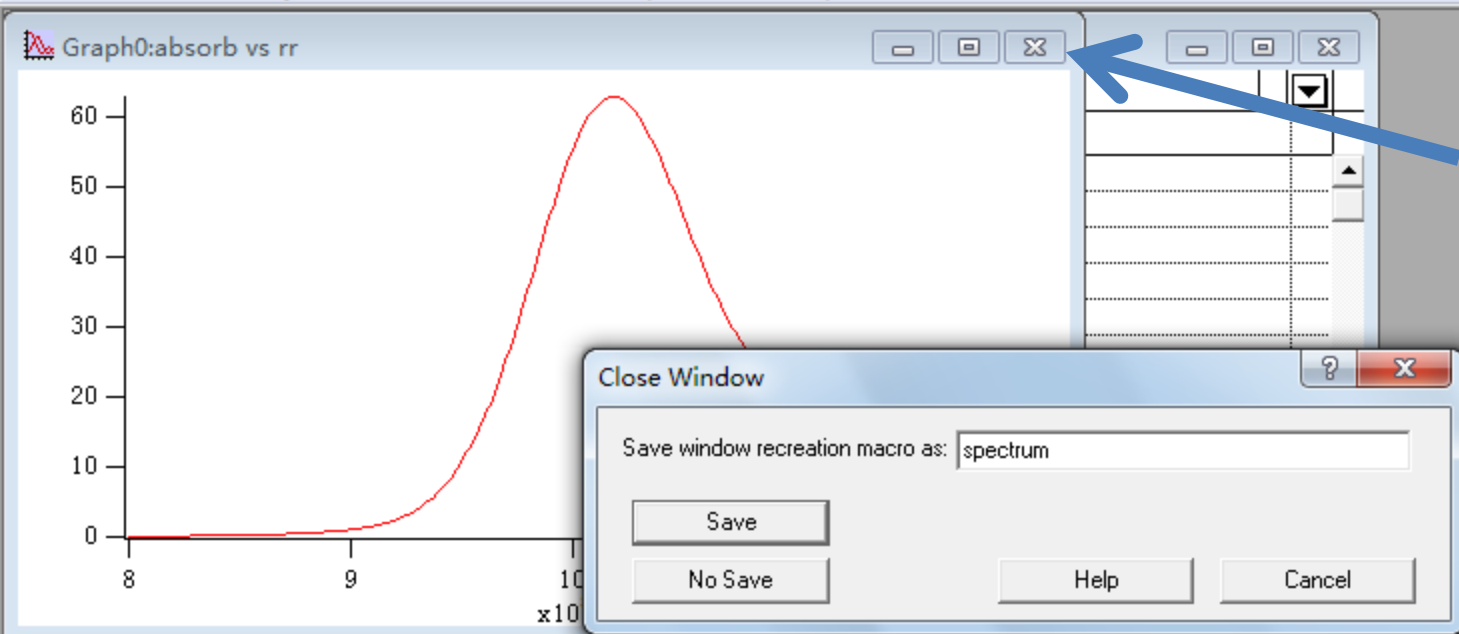
Point	absorb	rr
0	0.111871	8000
1	0.116967	8010
2	0.122121	8020
3	0.127326	8030
4	0.132574	8040
5	0.137856	8050
6	0.143166	8060
7	0.148495	8070
8	0.153836	8080
9	0.159183	8090
10	0.164528	8100

Untitled

```
*rename wave0 absorb  
*rename wave0 rr  
  
display absorb vs rr
```

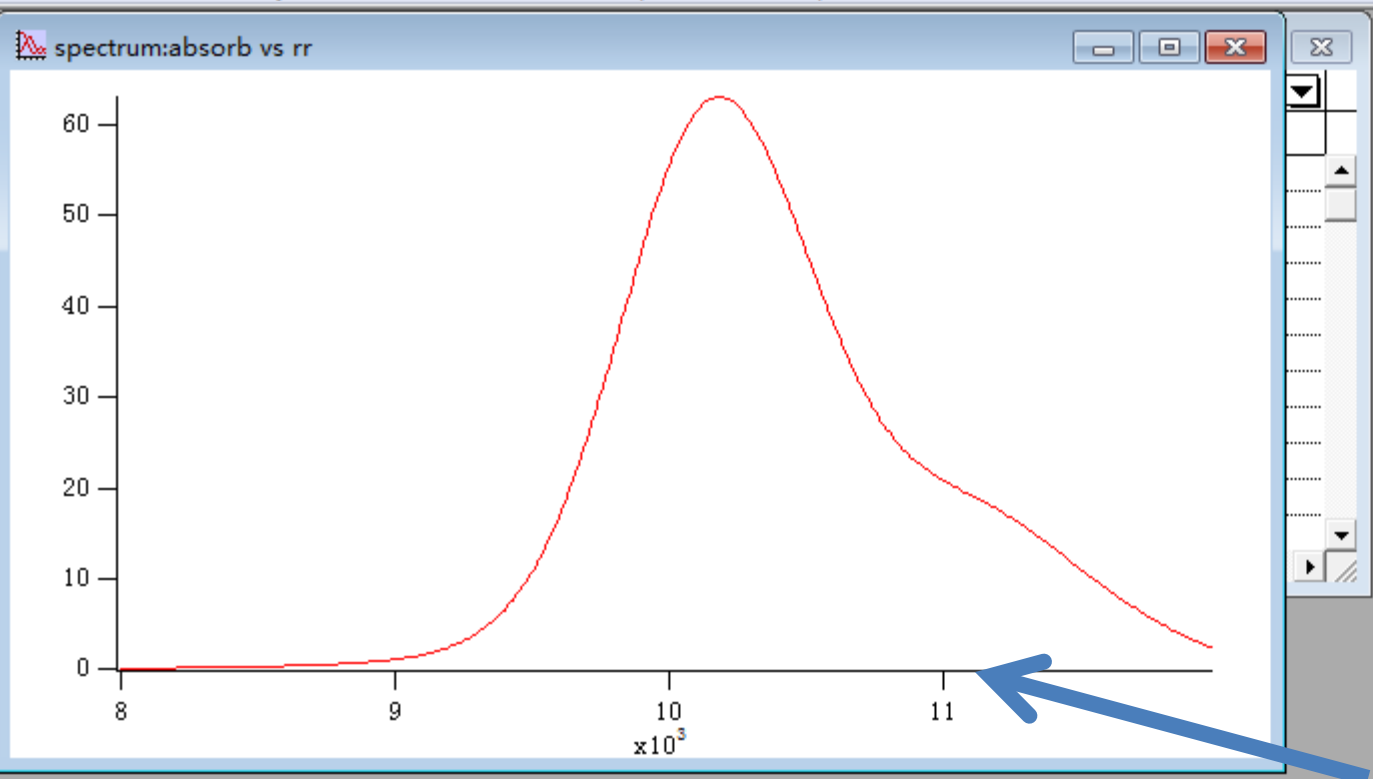
Saving Graphs

To close the graph and save it, click on the X in the upper right hand corner



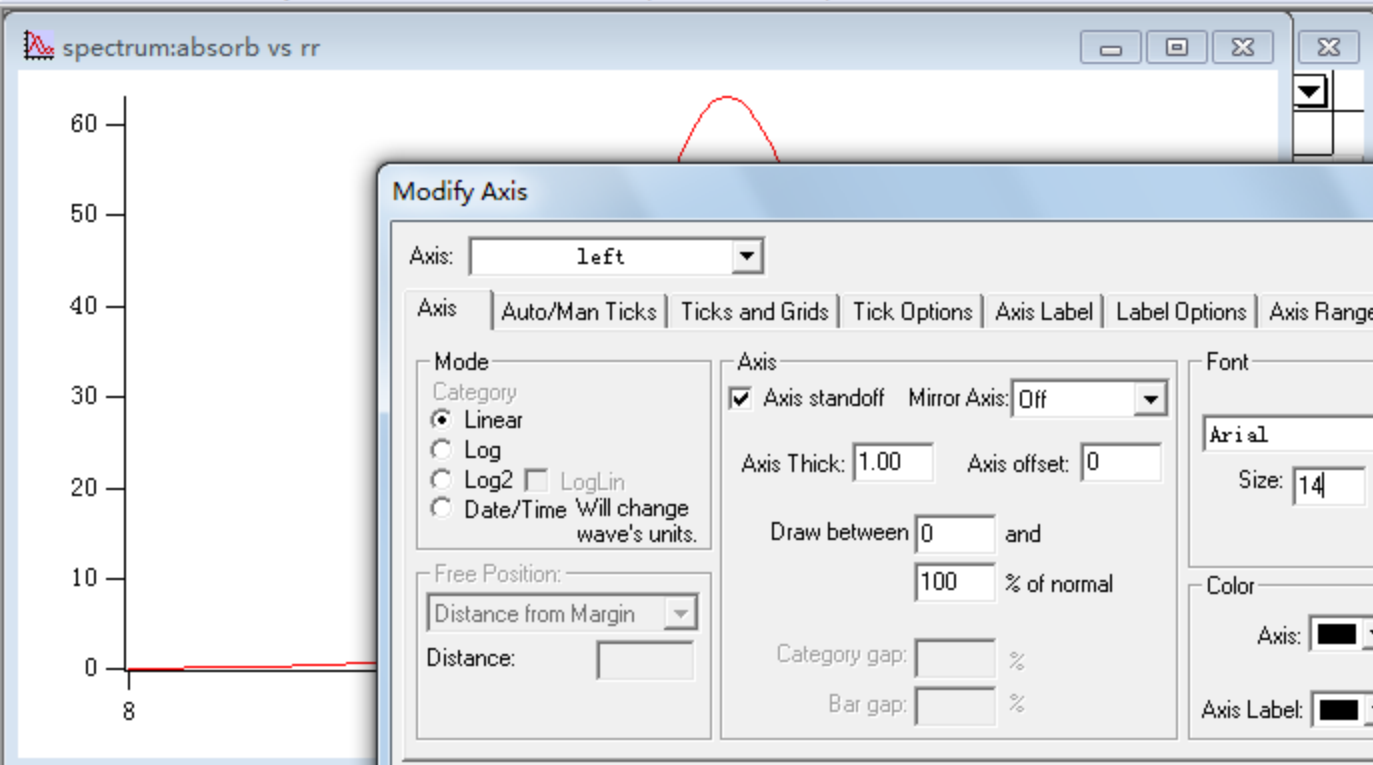
Click Here

```
Untitled  
*rename wave0 absorb  
*rename wave0 rr  
*display absorb vs rr
```



To modify axis
Click Here

```
Untitled  
*rename wave0 absorb  
*rename wave0 rr  
*display absorb vs rr  
*spectrum()
```



Modify Axis

Axis: **left** Live Update

Axis | Auto/Man Ticks | Ticks and Grids | Tick Options | Axis Label | Label Options | Axis Range

Mode

Category

Linear

Log

Log2 LogLin

Date/Time Will change wave's units.

Axis

Axis standoff Mirror Axis: **Off**

Axis Thick: **1.00** Axis offset: **0**

Draw between **0** and **100** % of normal

Category gap: %

Bar gap: %

Font

Arial

Size: **14**

Bold

Italic

Underline

Outline

Shadow

Free Position:

Distance from Margin **Distance:**

Color

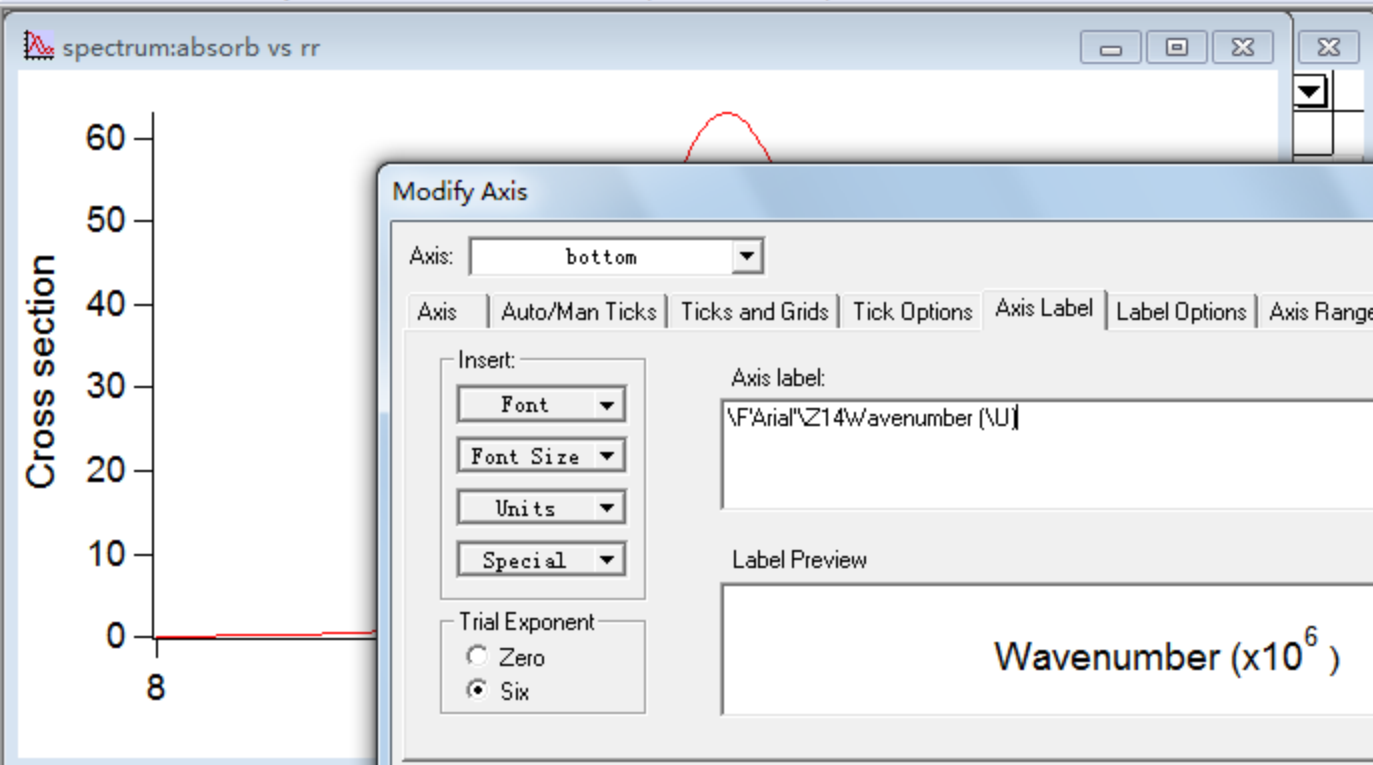
Axis: **Set All to Axis Color**

Axis Label: Tick Label:

ModifyGraph fSize=14, font="Arial"

Untitled

```
*rename wave0 absorb
*rename wave0 rr
*display absorb vs rr
*spectrum()
```



Modify Axis ? X

Axis: bottom Live Update

Axis | Auto/Man Ticks | Ticks and Grids | Tick Options | **Axis Label** | Label Options | Axis Range

Insert:

- Font ▼
- Font Size ▼
- Units ▼
- Special ▼

Trial Exponent:

- Zero
- Six

Axis label:

Label Preview:

Label bottom:

Do It | To Cmd Line | To Clip | Help | Cancel

```

Untitled
*rename wave0 absorb
*rename wave0 rr
*display absorb vs rr
*spectrum()
*ModifyGraph fSize=14,font="Arial"
*Label left "\Z14\F'Arial'Cross section";DelayUpdate
*Label bottom "\F'Arial'\Z14Wavenumber"
  
```

Fitting with Igor

Select Analysis/Curve Fitting

Choose a fitting function

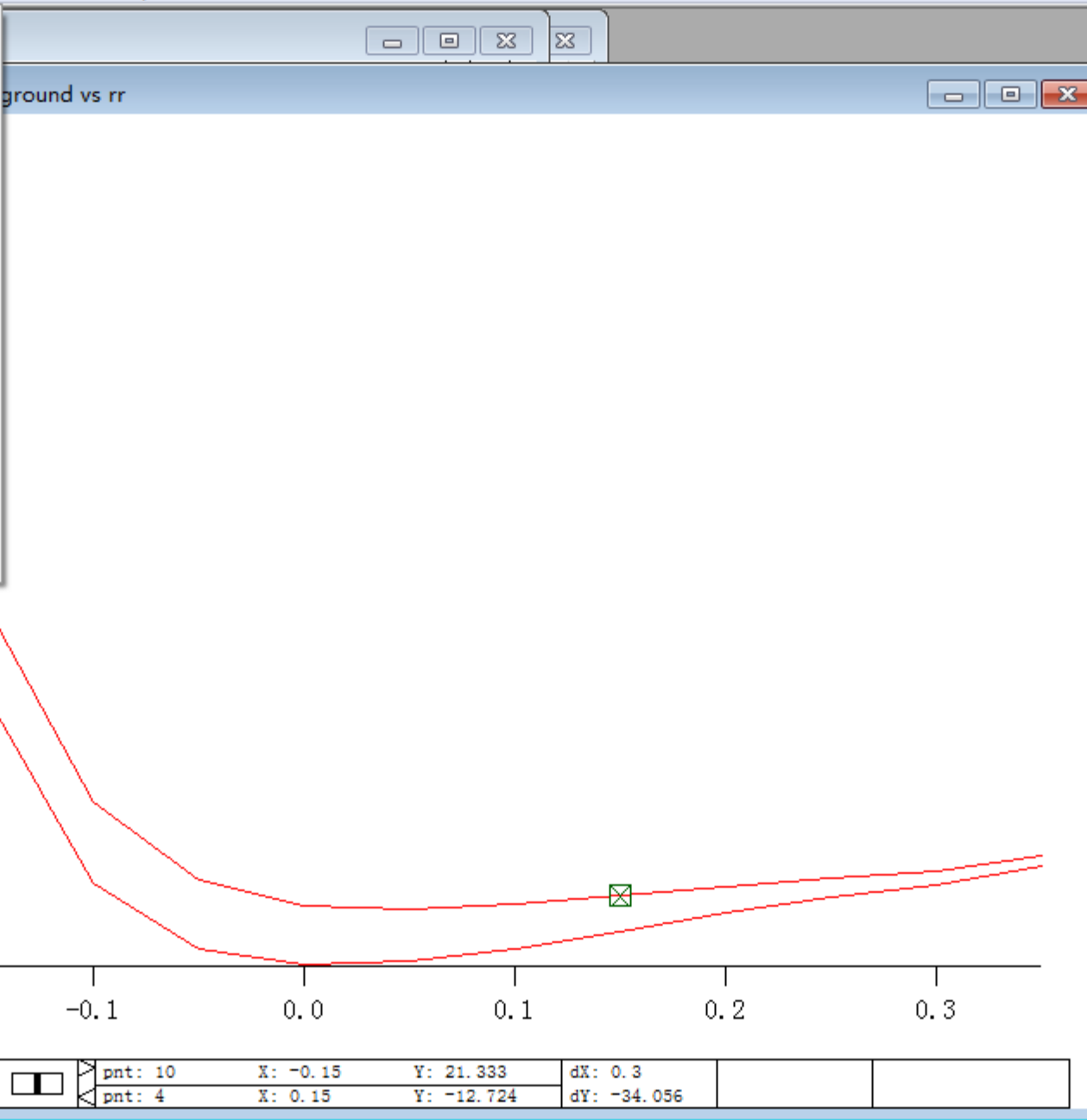
To use cursor type <Ctrl I>

Select [Data Options] to limit the range

Table0:pes,rr,
R12C0

Point
0
1
2
3
4
5
6
7
8
9
10
11
12

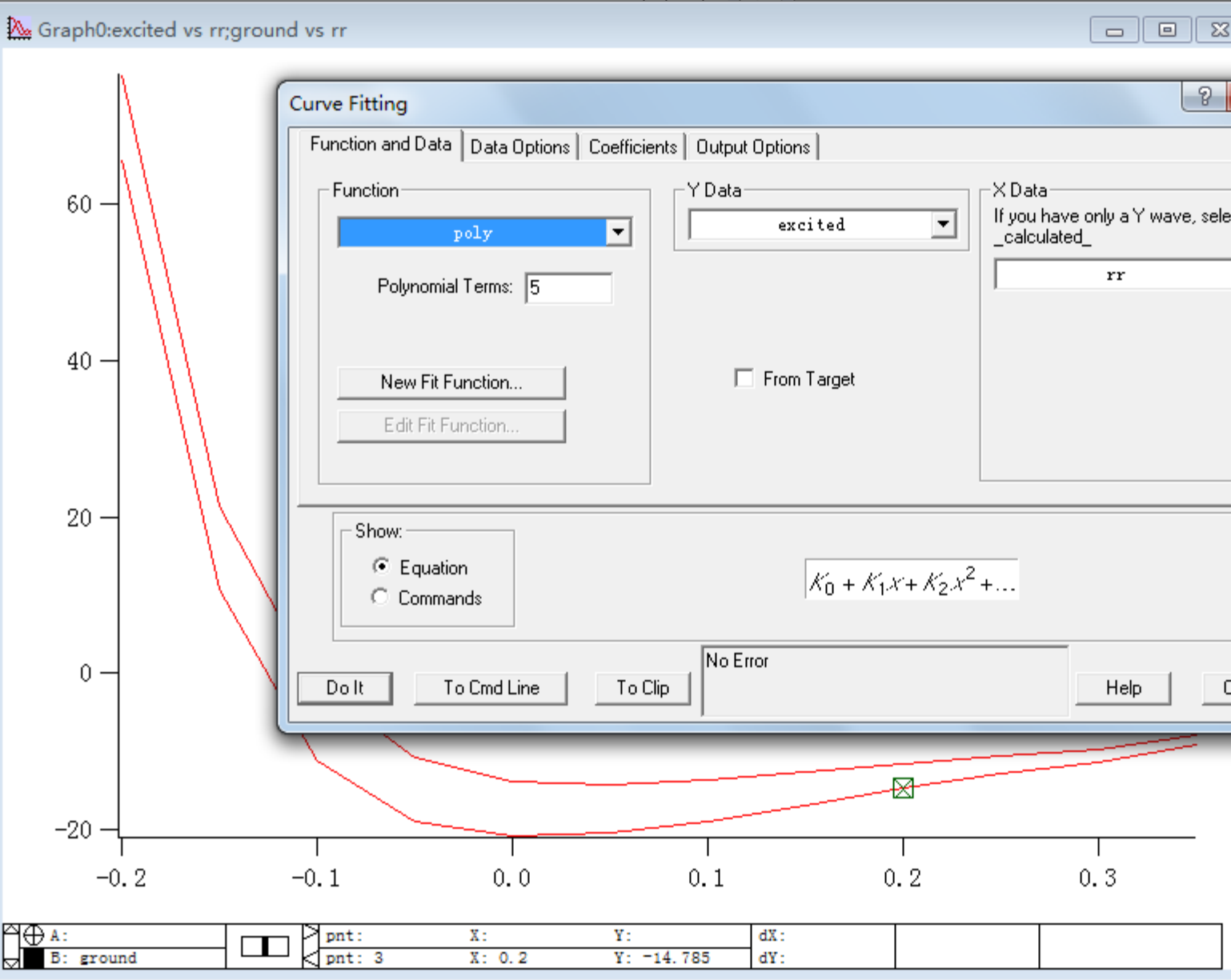
- Curve Fitting...
- Wave Stats...
- Fourier Transforms...
- Smooth...
- Hanning...
- Convolve...
- Correlate...
- Integrate...
- Differentiate...
- Histogram...
- Sort...
- Misc Operations ▶
- Compose Expression...
- Interpolate...
- Packages ▶



*SetAxis/A
*SetAxis/A
CurveFit poly 5, excit

Table0:pes,rr,excited,ground

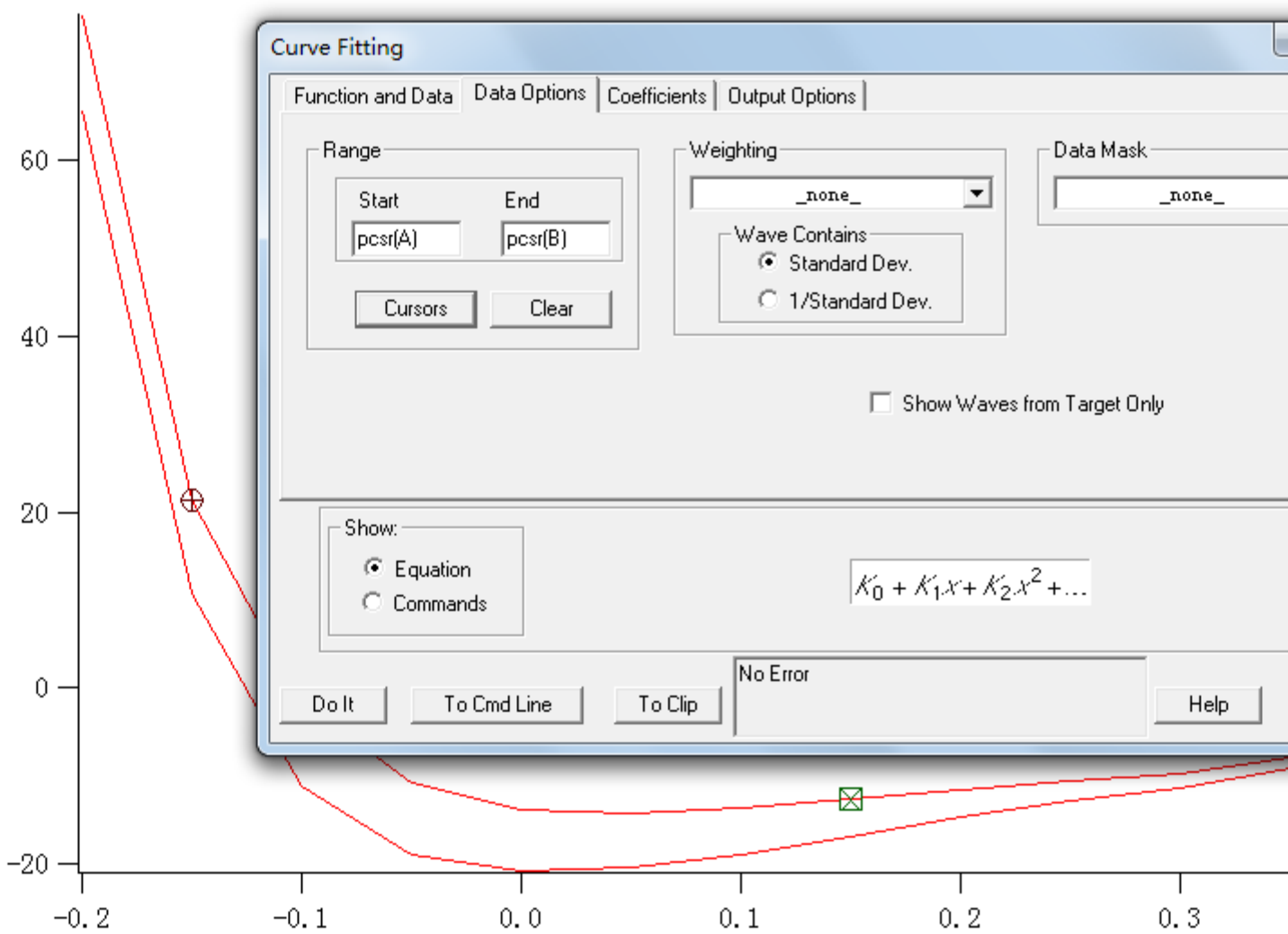
Point	pes
0	-1.90
1	-3.79
2	-4.83
3	-6.21
4	-7.82
5	-9.54
6	-11.1
7	-11.9
8	-10.4
9	-3.12
10	18.1
11	72.6
12	



*SetAxis/A
*SetAxis/A

A:		pnt:	X:	Y:	dX:	
B: ground		pnt: 3	X: 0.2	Y: -14.785	dY:	

Graph0:excited vs rr;ground vs rr



Curve Fitting

Function and Data | Data Options | Coefficients | Output Options

Range: Start pcsr(A), End pcsr(B) [Cursors] [Clear]

Weighting: Wave Contains: Standard Dev., 1/Standard Dev.

Data Mask:

Show Waves from Target Only

Show: Equation, Commands

$K_0 + K_1x + K_2x^2 + \dots$

No Error

[Do It] [To Cmd Line] [To Clip] [Help] [Cancel]

A: excited		pnt: 10	X: -0.15	Y: 21.333	dX: 0.3		
B: excited		pnt: 4	X: 0.15	Y: -12.724	dY: -34.056		