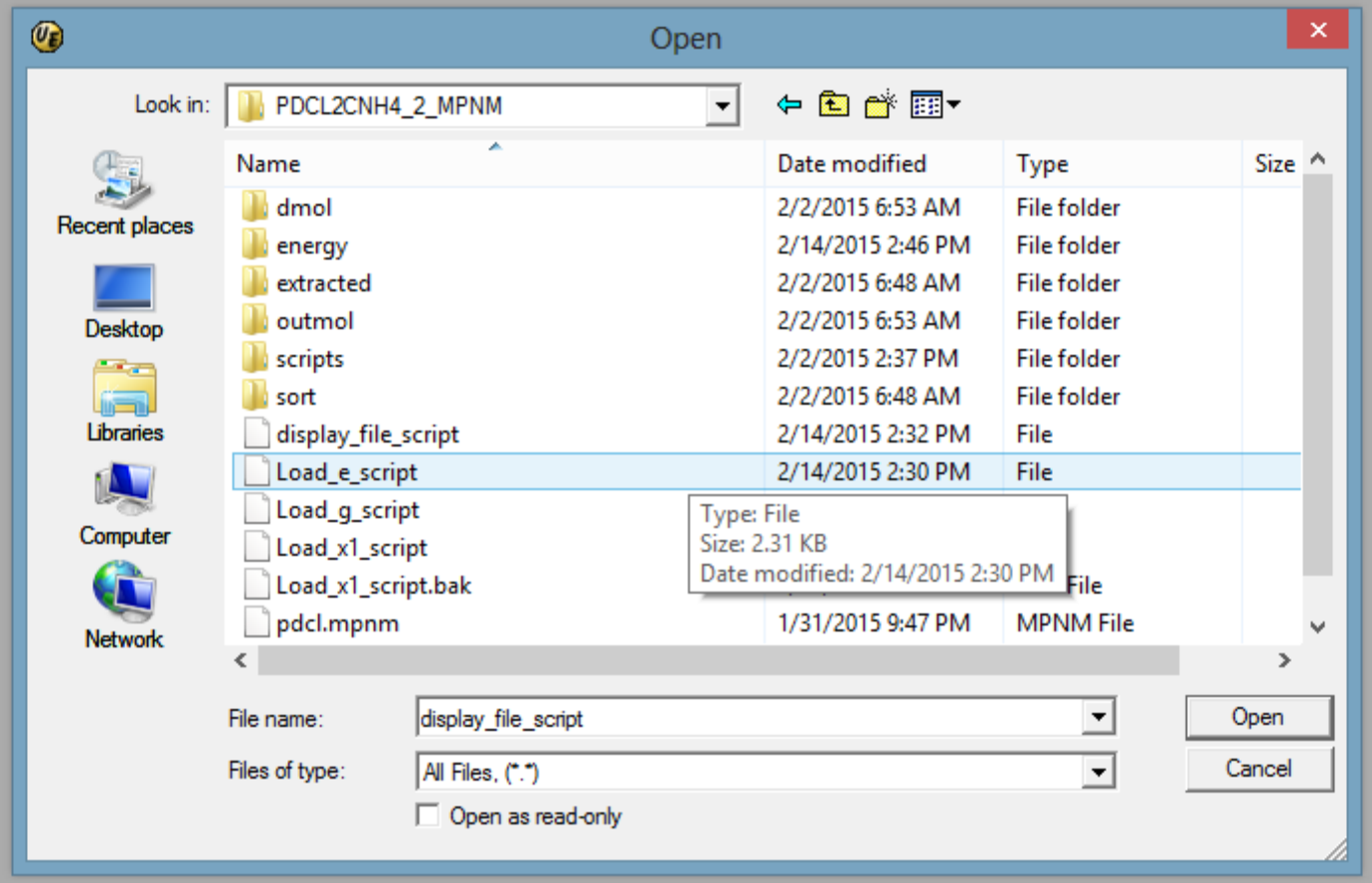
Plotting normal mode potential energy profiles

Using Igor Macros



To load files and plot them automatically, you need to edit the macros shown in this menu.

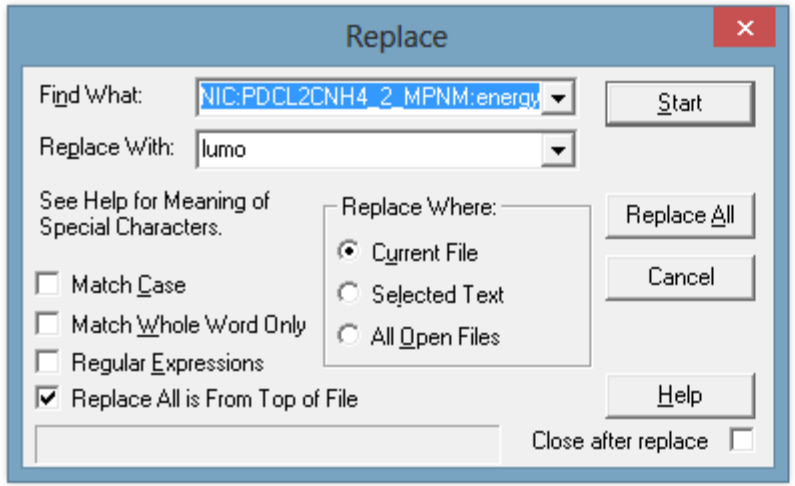
Edit Search Project View Format Column Macro Advanced Window Help

```
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_8.e"
me wave0 e8
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_9.e"
me wave0 e9
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_10.e"
me wave0 e10
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_11.e"
me wave0 e11
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_12.e"
me wave0 e12
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_13.e"
me wave0 e13
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_14.e"
me wave0 e14
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_15.e"
me wave0 e15
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_16.e"
me wave0 e16
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_17.e"
me wave0 e17
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_18.e"
me wave0 e18
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_19.e"
me wave0 e19
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_20.e"
me wave0 e20
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_21.e"
me wave0 e21
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_12.e"
me wave0 e22
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_23.e"
me wave0 e23
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_24.e"
me wave0 e24
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_25.e"
me wave0 e25
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_26.e"
me wave0 e26
```

This macro reads in the energy for each geometry calculated from the mpnm program. You will need to edit the macro to change the path and also the file name. The path is shown in blue.

Edit Search Project View Format Column Macro Advanced Window Help

```
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_8.homo"
me wave0 homo8
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_9.homo"
me wave0 homo9
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_10.homo"
me wave0 homo10
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_11.homo"
me wave0 homo11
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_12.homo"
me wave0 homo12
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_13.homo"
me wave0 homo13
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_14.homo"
me wave0 homo14
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_15.homo"
me wave0 homo15
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_16.homo"
me wave0 homo16
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_17.homo"
me wave0 homo17
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_18.homo"
me wave0 homo18
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_19.homo"
me wave0 homo19
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_20.homo"
me wave0 homo20
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_21.homo"
me wave0 homo21
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_22.homo"
me wave0 homo22
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_23.homo"
me wave0 homo23
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_24.homo"
me wave0 homo24
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_25.homo"
me wave0 homo25
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_26.homo"
me wave0 homo26
```

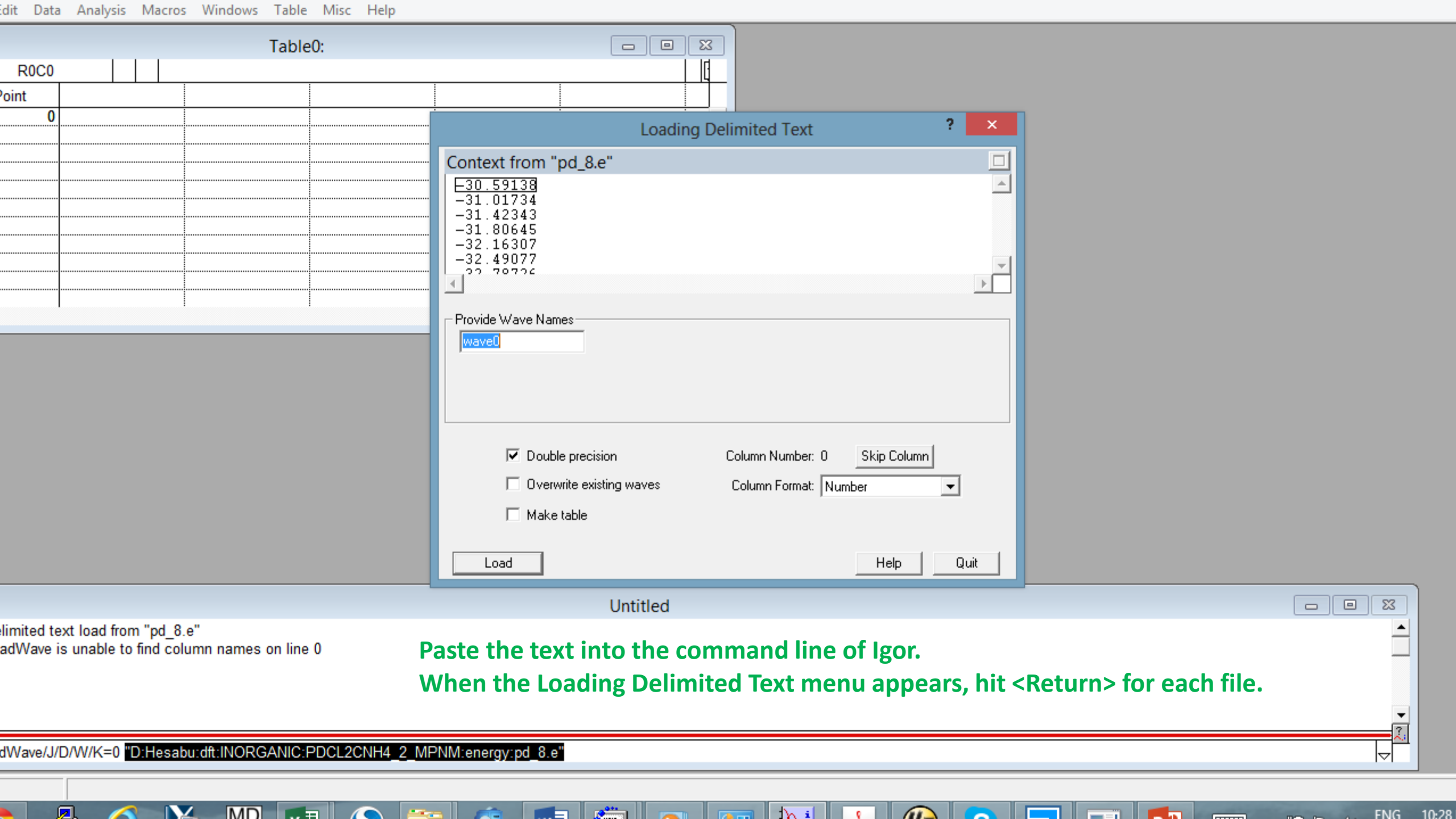


<ctrl R> calls the Replace menu in UltraEdit

Edit Search Project View Format Column Macro Advanced Window Help

```
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_8.e"
me wave0 e8
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_9.e"
me wave0 e9
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_10.e"
me wave0 e10
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_11.e"
me wave0 e11
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_12.e"
me wave0 e12
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_13.e"
me wave0 e13
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_14.e"
me wave0 e14
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_15.e"
me wave0 e15
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_16.e"
me wave0 e16
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_17.e"
me wave0 e17
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_18.e"
me wave0 e18
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_19.e"
me wave0 e19
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_20.e"
me wave0 e20
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_21.e"
me wave0 e21
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_12.e"
me wave0 e22
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_23.e"
me wave0 e23
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_24.e"
me wave0 e24
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_25.e"
me wave0 e25
Wave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_26.e"
me wave0 e26
```

Once you have edited the macro so the path name and the file names are correct, you select the text


Edit Data Analysis Macros Windows Table Misc Help
Table0:
R0C0
Point
0
Loading Delimited Text
Context from "pd_8.e"
-30.59138
-31.01734
-31.42343
-31.80645
-32.16307
-32.49077
Provide Wave Names
wave0
Double precision
Overwrite existing waves
Make table
Column Number: 0
Skip Column
Column Format:
Number
Load
Help
Quit
Untitled
limited text load from "pd_8.e"
adWave is unable to find column names on line 0
Paste the text into the command line of Igor.
When the Loading Delimited Text menu appears, hit <Return> for each file.
dWave/J/D/W/K=0 "D:Hesabu:dft:INORGANIC:PDCL2CNH4_2_MPNM:energy:pd_8.e"

You will need to read in:

1. **The energy**
2. **The HOMO**
3. **The LUMO**

This is the minimum information required, but you may also wave to look at higher states.

The next macro will calculate the energy of the excited state

Excited = Energy + LUMO – HOMO

e Edit Search Project View Format Column Macro Advanced Window Help

```
.cate e8 t8
8-homo8+lumo8
.cate e9 t9
9-homo9+lumo9
.cate e10 t10
e10-homo10+lumo10
.cate e11 t11
e11-homo11+lumo11
.cate e12 t12
e12-homo12+lumo12
.cate e13 t13
e13-homo13+lumo13
.cate e14 t14
e14-homo14+lumo14
.cate e15 t15
e15-homo15+lumo15
.cate e16 t16
e16-homo16+lumo16
.cate e17 t17
e17-homo17+lumo17
.cate e18 t18
e18-homo18+lumo18
.cate e19 t19
e19-homo19+lumo19
.cate e20 t20
e20-homo20+lumo20
.cate e21 t21
e21-homo21+lumo21
.cate e22 t22
e22-homo22+lumo22
.cate e23 t23
e23-homo23+lumo23
.cate e24 t24
e24-homo24+lumo24
.cate e25 t25
e25-homo25+lumo25
.cate e26 t26
e26-homo26+lumo26
```

This macro will calculate the excited state potential energy profile for each normal mode. It will also plot the energy profiles.

Edit Data Analysis Macros Windows Table Misc Help

Table0:

R0C0

Point

0

display Error

expected wave name

OK

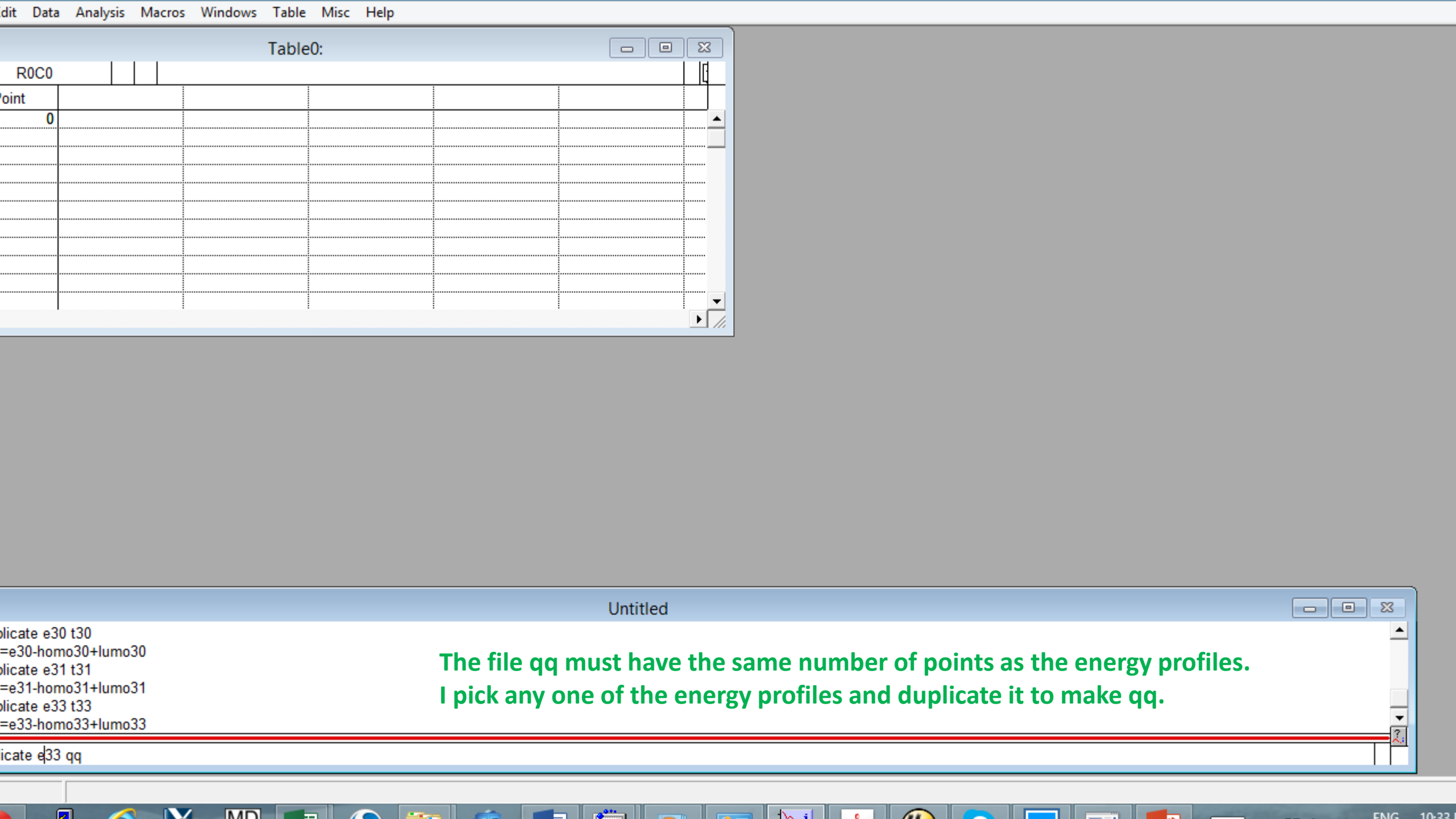
Explain Operation

Untitled

licate e30 t30
=e30-homo30+lumo30
licate e31 t31
=e31-homo31+lumo31
licate e33 t33
=e33-homo33+lumo33

lay e8,t8 vs qq

I forgot to define a file that represents the X-axis, i.e. the nuclear coordinate motion. I call this file qq (since single letters are often reserved in Igor).


Edit Data Analysis Macros Windows Table Misc Help
Table0:
R0C0
Point
0
Untitled
plicate e30 t30
=e30-homo30+lumo30
plicate e31 t31
=e31-homo31+lumo31
plicate e33 t33
=e33-homo33+lumo33
icate e33 qq
The file qq must have the same number of points as the energy profiles.
I pick any one of the energy profiles and duplicate it to make qq.

Edit Data Analysis Macros Windows Table Misc Help

Table1:qq

R0C0	-2
Point	qq
0	-2
1	-1.9
2	-1.8
3	-1.7
4	-1.6
5	-1.5
6	-1.4
7	-1.3
8	-1.2
9	-1.1
10	-1

At the end of the operations you see that qq ranges from -2 to 2, which was my range for nuclear motion used in mpnm.

Untitled

```
=e33-homo33+lumo33
licate e33 qq
t qq
=x
=20
=10
```

Here I have combined several steps. I use the edit command just so I can see The results . I set qq = x, which means that qq is an array of integers from 0 to N.

Edit Data Analysis Macros Windows Table Misc Help

Table1:qq

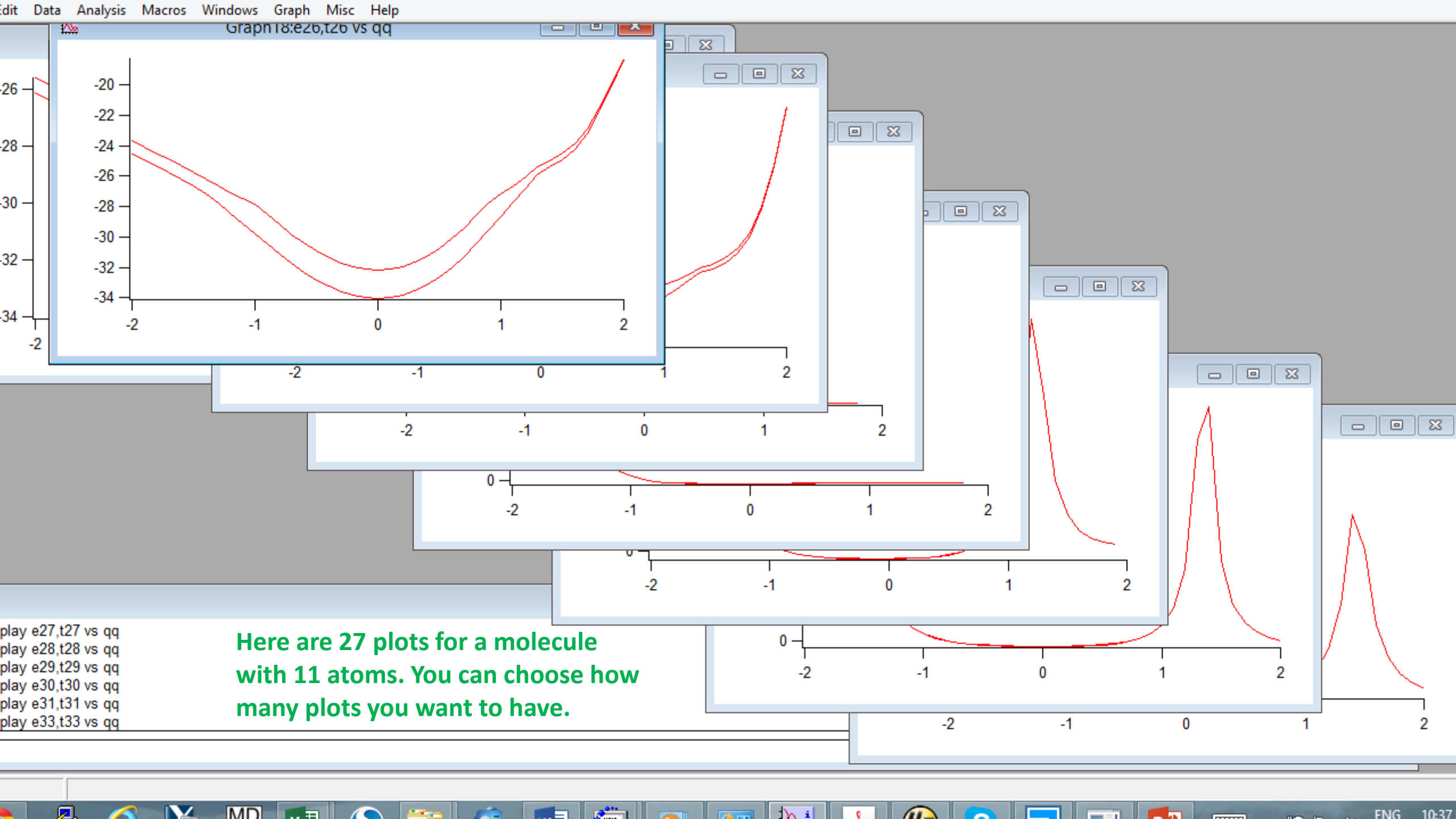
R0C0 | -2

Point	qq
7	-1.3
8	-1.2
9	-1.1
10	-1
11	-0.9
12	-0.8
13	-0.7
14	-0.6
15	-0.5
16	-0.4
17	-0.3
18	-0.2
19	-0.1
20	0
21	0.1
22	0.2
23	0.3
24	0.4
25	0.5
26	0.6
27	0.7
28	0.8
29	0.9
30	1
31	1.1
32	1.2
33	1.3
34	1.4
35	1.5
36	1.6
37	1.7
38	1.8
39	1.9
40	2
41	

This the rest of qq

```
display e8,t8 vs qq
display e9,t9 vs qq
display e10,t10 vs qq
display e11,t11 vs qq
display e12,t12 vs qq
display e13,t13 vs qq
display e14,t14 vs qq
display e15,t15 vs qq
display e16,t16 vs qq
display e17,t17 vs qq
display e18,t18 vs qq
display e19,t19 vs qq
display e20,t20 vs qq
display e21,t21 vs qq
display e22,t22 vs qq
display e23,t23 vs qq
display e24,t24 vs qq
display e25,t25 vs qq
display e26,t26 vs qq
display e27,t27 vs qq
display e28,t28 vs qq
display e29,t29 vs qq
display e30,t30 vs qq
display e31,t31 vs qq
display e33,t33 vs qq
```

This is the final part of the script that I will paste into Igor. It just plots the ground and excited state energy profiles vs. nuclear motion. It does this using one key stroke.


Edit Data Analysis Macros Windows Graph Misc Help
Graph18:e26,t26 vs qq
play e27,t27 vs qq
play e28,t28 vs qq
play e29,t29 vs qq
play e30,t30 vs qq
play e31,t31 vs qq
play e33,t33 vs qq
Here are 27 plots for a molecule with 11 atoms. You can choose how many plots you want to have.