Converting “sticks” into spectra

Use the programs

Abs_spec.f (spectra in wavelength from 1 to 1000 nm)
Abs_cm_1_spec.f (spectra in wave number from 1 to 40000 cm-1)
Ir_spec.f (infrared spectra from 1 to 4000 cm-1)

You may compile
$ f77 abs_spec.f –o abs_spec

Same for the others.
The programs look for input from input.dat

Input.dat
#of points
#omega1 #intensity1
#omega2 #intensity2
#omega3 #intensity3
…..

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[franzen@login03 for]$ ls
abs_cm_1_spec  abs_cm_1_spec.f  abs_spec  abs_spec.f  input.dat  ir_spec.f  output.dat
[franzen@login03 for]$ vi input.dat
```

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12500  1.7
14100 2.1
16200 3.4
17400 1.2
23400 10.4
25000 1.3
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"input.dat" 7L, 64C
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[franzen@login03 for]$ abs_spec < input.dat
```

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[franzen@login03 for]$ abs_spec < input.dat
 Use redirect to input data: abs_spec < data.inp
 Enter Number of transitions:
  12500.  1.7
  14100.  2.1
  16200.  3.4
  17400.  1.2
  23400.  10.4
  25000.  1.3
 Error in output file
[franzen@login03 for]$
```

The program will write output.dat

It will not write over the old file. If you want to overwrite it the delete it.

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 Use redirect to input data: abs_spec < data.inp
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  12500.  1.7
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  16200.  3.4
  17400.  1.2
  23400.  10.4
  25000.  1.3
 Error in output file
[franzen@login03 for]$
```

Now it ran successfully and generated output.dat
You may plot this file in Excel, Origin, Igor etc.

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