

Computers in Chemistry – Lecture XII

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Get this lecture online

- Please go to: <http://qc.chem.nagoya-u.ac.jp>
- Click on “Teaching”
- Click on “PPT” link of “12.1 Lecture XII – Data Visualization with FORTRAN and Gnuplot”
userid: **qcguest**, password: **qcigf!**

11.5 Example data: [benzene.xyz](#), [h2o-ir.dat](#)
12.1 Lecture XII - Data Visualization with FORTRAN and Gnuplot (PDF)
12.2 Example data: [sulflower.out](#), [sulflower-ir.dat](#)

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Applications of FORTRAN to Chemistry I

- Download program “spectrum.f90” from <http://qc.chem.nagoya-u.ac.jp/teaching> (Lecture 11), compile, and test using the “h2o-ir.dat” example (also available on the website)
- h2o-ir.dat (raw data, computed IR frequencies and intensities, **input**):

1713.0153	75.7994
3727.3732	1.6952
3849.4717	19.3975

Wavenumber (cm⁻¹) IR intensities (km/mol)

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Applications of FORTRAN to Chemistry II

- In X11 Terminal, do the following:
 - `cd “Downloads”`
 - `cat h2o-ir.dat` (will show file contents)
 - `cat spectrum.f90` (look at program)
 - `gfortran -o spectrum.x spectrum.f90`
(compile program)
 - `./spectrum.x` (run program)
- Please give number of vibrations:
3
Please give name of data file:
h2o-ir.dat
Please input sigma value:
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Applications of FORTRAN to Chemistry III

```
• ls spectrum.out (check if file is there)
• cat spectrum.out (will show file contents)
  1  0.000000
  2  0.000000
  3  0.000000
  4  0.000000
  5  0.000000
  6  0.000000
  7  0.000000
  8  0.000000
  9  0.000000
 10  0.000000
 11  0.000000
...
 1709  75.12350
 1710  75.41750
 1711  75.62857
 1712  75.75600
 1713  75.79939
 1714  75.75858
 1715  75.63370
 1716  75.42517
 1717  75.13370
...
 4993  0.000000
 4994  0.000000
 4995  0.000000
 4996  0.000000
 4997  0.000000
 4998  0.000000
 4999  0.000000
 5000  0.000000
```

Continuous IR spectrum,
"recorded" in intervals of 1
cm⁻¹

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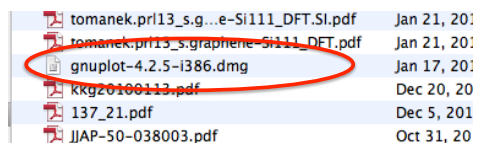
Applications of FORTRAN to Chemistry IV

- Plot the spectra for various choices of σ using the GNU PLOT software, also available on <http://qc.chem.nagoya-u.ac.jp/teaching>
 - 11.1 Lecture XI - File Input/Output in FORTRAN (PDF)
 - 11.2 Solution to Assignment 7: rotvec.f90
 - 11.3 Example programs: rotmol.f90, spectrum.f90
 - 11.4 Gnuplot for Mac OS **gnuplot-4.2.5-i386.dmg**
 - 11.5 Example data: benzene.xyz, n2o-ir.dat
- Save "disk image" (.dmg) file under "Downloads"
- Open Finder Window

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Applications of FORTRAN to Chemistry V

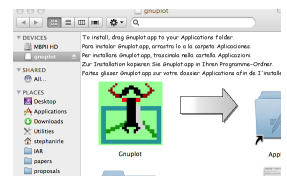
- Open Finder Window
- "Double-click" on "gnuplot-4-2.5-i38.dmg" (will possibly print a warning)

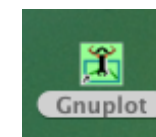


- A new window appears:

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Applications of FORTRAN to Chemistry VI

- A new window appears:
- Point mouse arrow and drag "Gnuplot" icon to Desktop
- On Desktop, Double-click" icon "Gnuplot"



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Applications of FORTRAN to Chemistry VII

- A new X11 terminal window appears:

```
Terminal — gnuplot-4.2.5 — 80x24
exec '/Applications/Gnuplot.app/Contents/Resources/bin/gnuplot'
Last login: Thu Jan 17 05:34:34 on ttys003
You have new mail.
Irlc-MacBookPro[1] exec '/Applications/Gnuplot.app/Contents/Resources/bin/gnuplot'
t'

G N U P L O T
Version 4.2 patchlevel 5
Last modified Mar 2009
System: Darwin 10.8.0

Copyright (C) 1986 - 1993, 1998, 2004, 2007 - 2009
Thomas Williams, Colin Kelley and many others

Type 'help' to access the on-line reference manual.
The gnuplot FAQ is available from http://www.gnuplot.info/faq/

Send bug reports and suggestions to <http://sourceforge.net/projects/gnu
plot>

Terminal type set to 'aqua'
gnuplot>
```

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Applications of FORTRAN to Chemistry VIII

- At the gnuplot> prompt, enter:
- cd 'Downloads', (" are important!)
- plot 'spectrum.out'

```
Terminal type set to 'aqua'
gnuplot> cd Downloads
undefined variable: Downloads

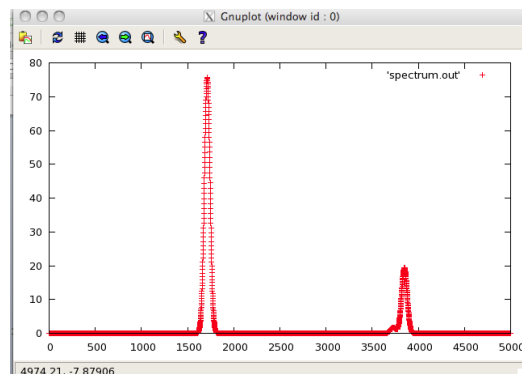
gnuplot> cd 'Downloads'
gnuplot> plot 'spectrum.out'
```

- A new window opens:

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Applications of FORTRAN to Chemistry IX

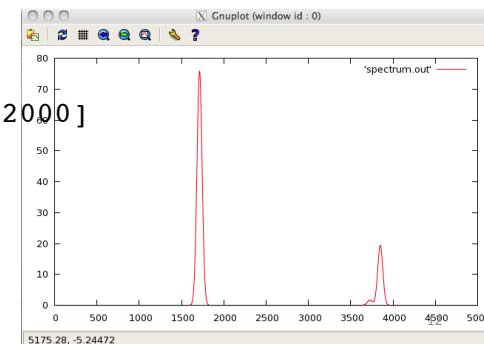
- A new window opens:



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Applications of FORTRAN to Chemistry X

- To plot a continuous line, enter the following at the gnuplot> prompt:
- set style data lines
- plot 'spectrum.out'
- The plot changes to this:
- Try the following:
- set xrange [1000:2000]

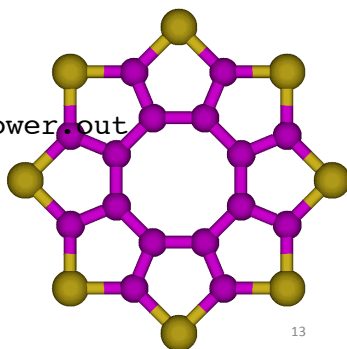
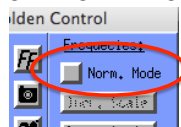


Applications of FORTRAN to Chemistry XI

- Practice: Download “sulflower.out” from <http://qc.chem.nagoya-u.ac.jp/teaching>

11.5 Example data: [benzene.xyz](#), [h2o-ir.dat](#)
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- In X11 terminal, do the following:
- cd Downloads
- ./molden4.8.macosX sulflower.out
- In Molden control window, click on “Norm. Mode”



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Applications of FORTRAN to Chemistry XIII

- How to invert the intensity scale?
- Download IR wavenumber and intensities from website, file “sulflower-ir.dat”

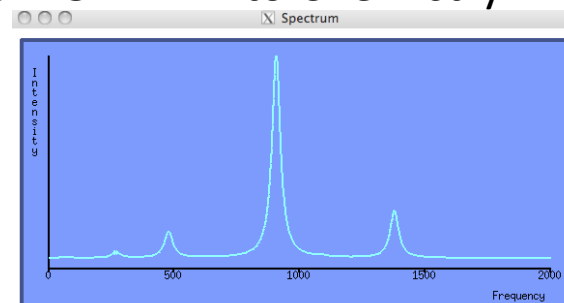
11.5 Example data: [benzene.xyz](#), [h2o-ir.dat](#)
 12.1 Lecture XII - Data Visualization with FORTRAN and Gnuplot (PDF)
 12.2 Example data: [sulflower.out](#), [sulflower-ir.dat](#)

- Answer: modify ‘spectrum.f90’ to print negative intensities
- This concludes today’s lecture and this course.
- Note: February 7: Exam, “Open Book” style, that means you can use ALL HOMEWORK, lecture notes, internet, etc.**

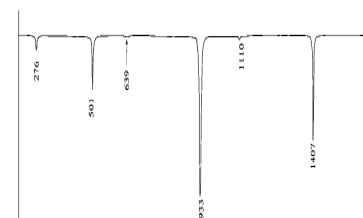
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Applications of FORTRAN to Chemistry XII

- The following window appears:



- Compare to experiment IR spectrum (J. Phys. Chem. A 2008, p. 10949):



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