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

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)

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:
30
```

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}

Applications of FORTRAN to Chemistry IV

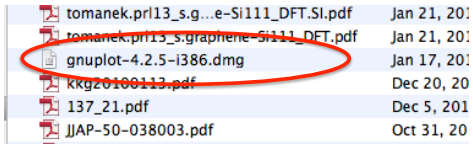
- Plot the spectra for various choices of σ using the GNUPLOT software, also available on http://qc.chem.nagoya-u.ac.jp/teaching

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 X: gnuplot-4.2.5-i386.dmg
11.5 Example data: benzene.xyz, h2o-ir.dat

- Save "disk image" (.dmg) file under "Downloads"
- Open Finder Window

Applications of FORTRAN to Chemistry V

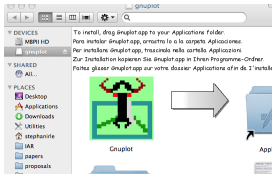
- Open Finder Window
- "Double-click" on "gnuplot-4-2.5-i38.dmg" (will possibly print a warning)



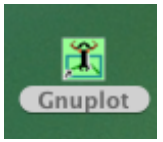
- A new window appears:

Applications of FORTRAN to Chemistry VI

- A new window appears:

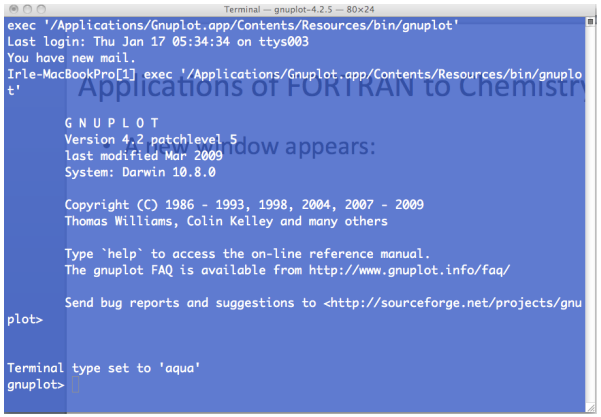


- Point mouse arrow and drag "Gnuplot" icon to Desktop
- On Desktop, Double-click" icon "Gnuplot"



Applications of FORTRAN to Chemistry VII

- A new X11 terminal window appears:



Applications of FORTRAN to Chemistry VIII

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

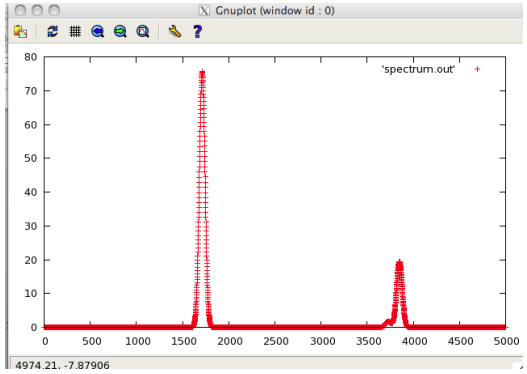
```
Terminal type set to 'aqua'
gnuplot> cd Downloads
         undefined variable: Downloads

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

- A new window opens:

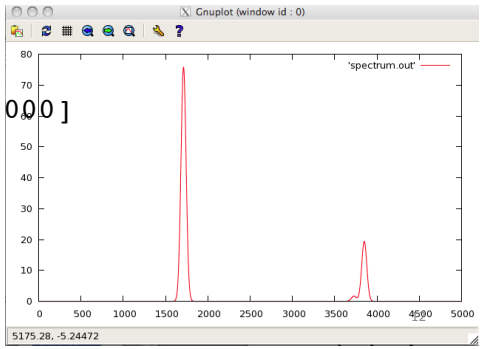
Applications of FORTRAN to Chemistry IX

- A new window opens:



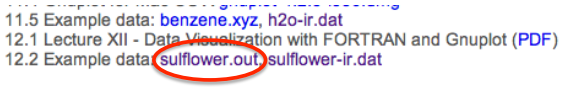
Applications of FORTRAN to Chemistry X

- 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]`

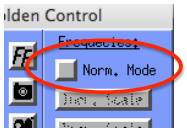


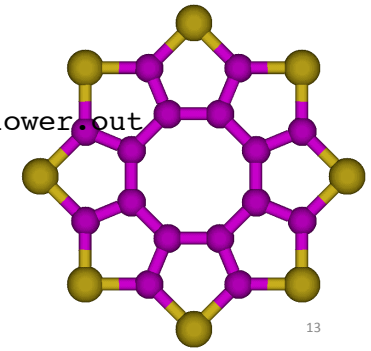
Applications of FORTRAN to Chemistry XI

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



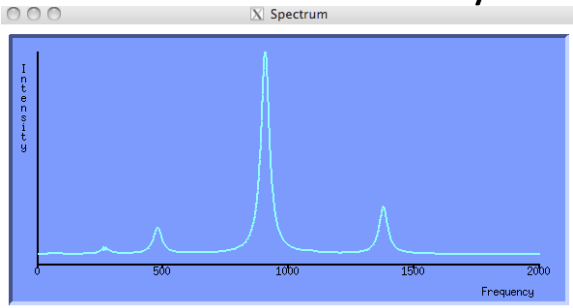
- In X11 terminal, do the following:
- `cd Downloads`
- `./molden4.8.macosX sulflower.out`
- In Molden control window, click on “Norm. Mode”



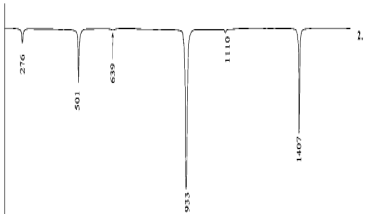


Applications of FORTRAN to Chemistry XII

- The following window appears:

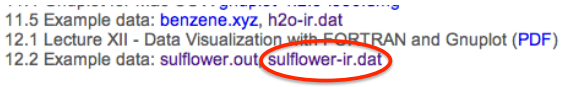


- Compare to experiment IR spectrum (J. Phys. Chem. A 2008, p. 10949):



Applications of FORTRAN to Chemistry XIII

- How to invert the intensity scale?
- Download IR wavenumber and intensities from website, file “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.**