Introduction to GaussView and Gaussian

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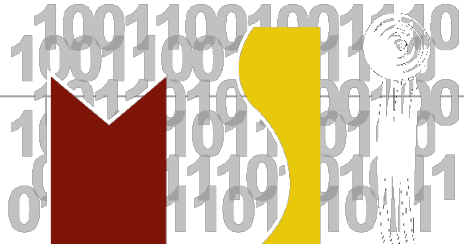

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- Description of Both Programs
- How to Create Input Files (with GaussView)
- How to Submit Calculations
- How to Visualize Output

Gaussian 03:

an electronic structure package capable of predicting many properties of atoms, molecules, and reactive systems

e.g.

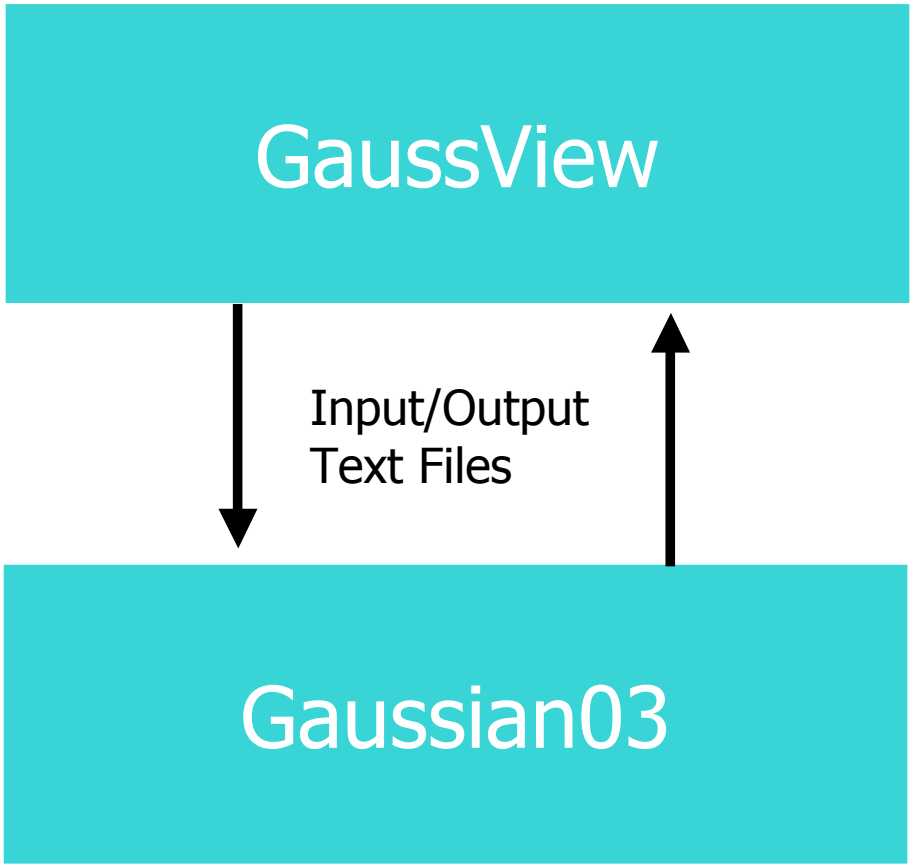
- Energies
- Structures
- Vibrational frequencies

utilizing *ab initio*, density functional theory, semi-empirical, molecular mechanics, and hybrid methods.

GaussView:

graphical interface for Gaussian 03

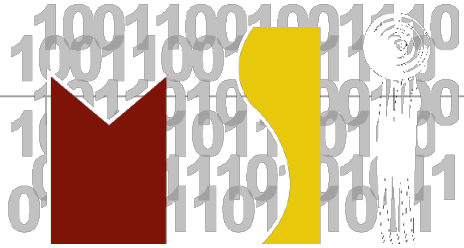
- build molecules or reactive systems
- setup Gaussian 03 input files
- graphically examine results



Visualization

Electronic Structure Calculations

Calculations with Gaussian



Types of Calculations

- single point energy and properties (electron density, dipole moment, …)
- geometry optimization
- frequency
- reaction path following

Levels of Theory Available:

- semi-empirical
  - AM1, PM3, MNDO, …
- density functional theory
  - B3LYP, MPW1PW91, …
- *ab initio*
  - HF, MP2, CCSD, CCSD(T), …
- hybrid
  - G2, G3, …

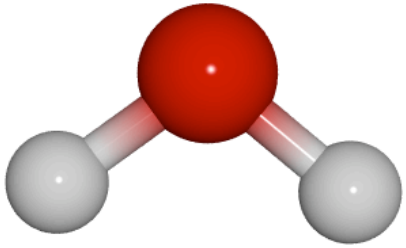
The level of theory is the set of underlying approximations used to describe the chemical system. Higher levels of theory are often more accurate however they come at much greater computational cost.

Basis Sets Available:

- Pople-type
  - 3-21G, 6-31G, 6-311G(d,p), …
- Dunning
  - cc-pVDZ, aug-cc-pVTZ, …
- Huzinaga and Others
  - MIDIX, …
- User-defined

Basis sets are used for most calculations in Gaussian. They are a set of functions that are used to describe electronic wavefunctions.

Creating Input Files for Gaussian



Water Optimization Input File

```
%mem=32mb
#p hf/6-31g opt

hf/6-31g optimization of water

0  1
o
h  1  oh
h  1  oh  2  ahoh

oh=0.9
ahoh=104.0
```

system resources

computational model
type of calculation

title

charge & multiplicity

structure definition
(z-matrix)

variable values

Spin multiplicity:

multiplicity = *n* + 1

where *n* = # of unpaired electrons

Building with GaussView:

- Instead of typing all the coordinates, theory, basis set, etc., we can use GaussView.
- The calculation is specified by pointing and clicking to build the molecule, and using pull-down menus to select the calculation type, level of theory and basis set.
- GaussView generates the Gaussian input file, and can run Gaussian without ever returning to the Unix prompt.
- GaussView can also be used to read Gaussian output files and visualize the results.

Getting Started with GaussView:

- Login remotely

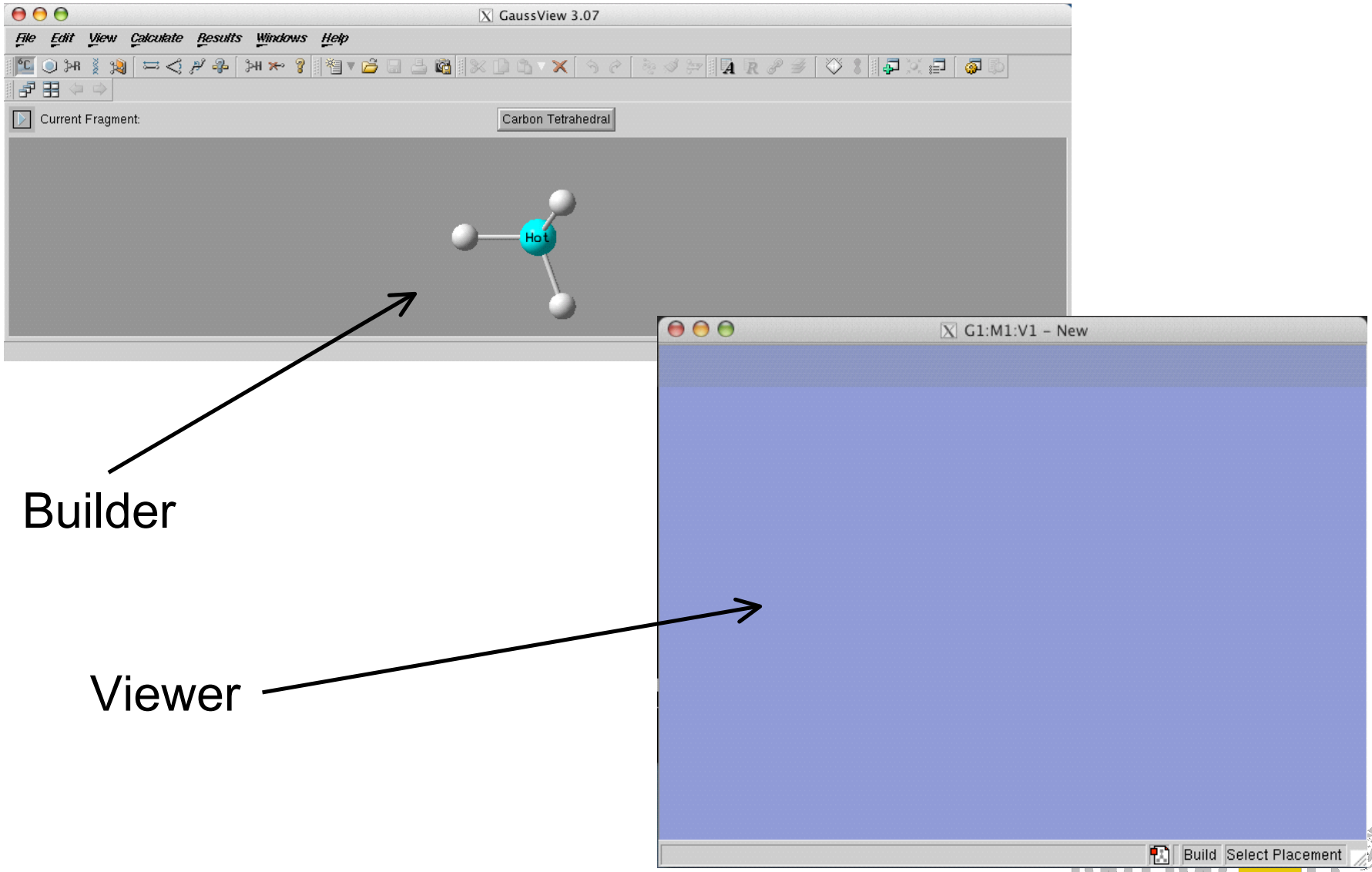
  ssh -X sp.msi.umn.edu

- Load Gaussian/GaussView module

  module add g03

- Launch GaussView

  gv

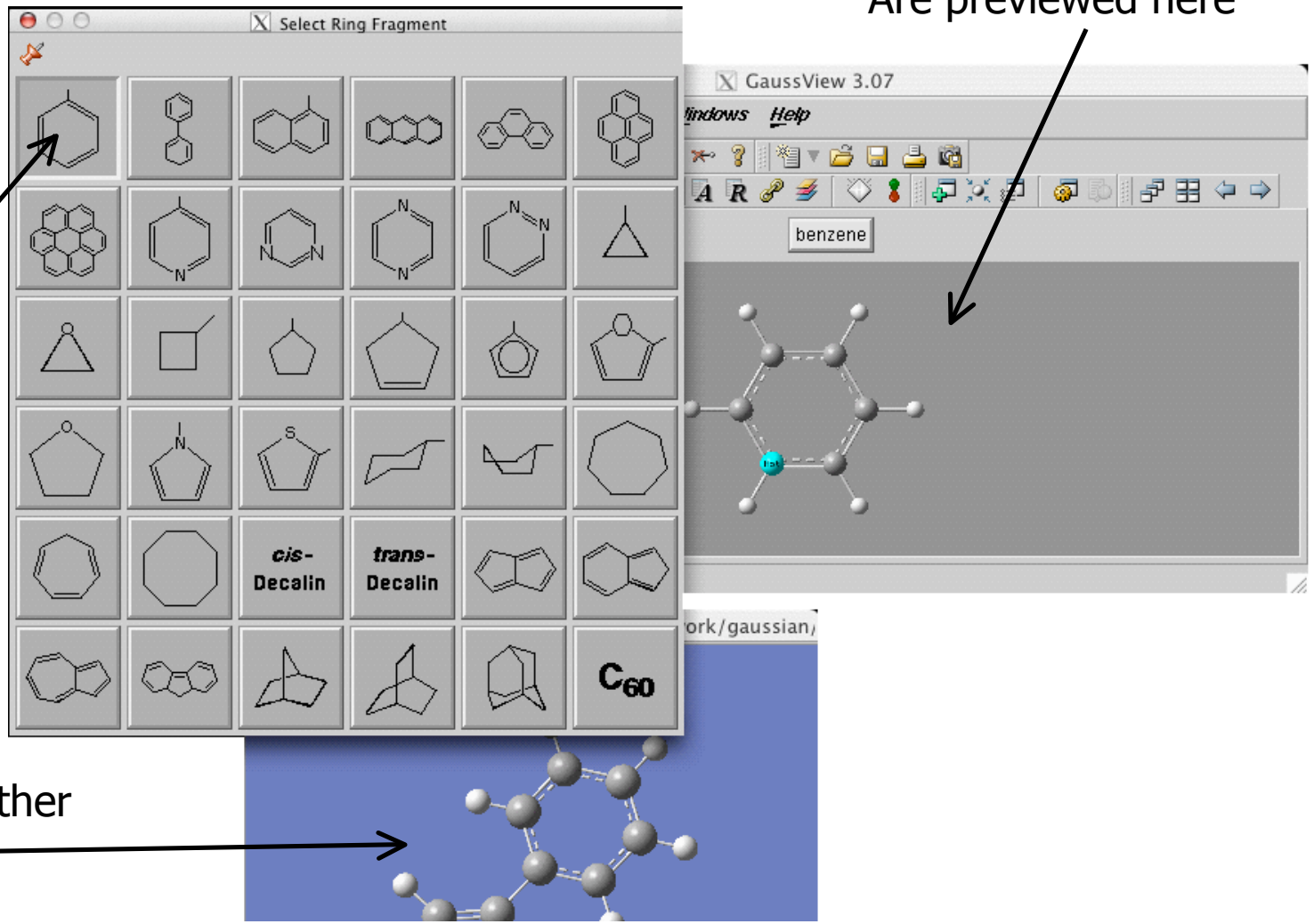

GaussView 3.07
File Edit View Calculate Results Windows Help
Current Fragment:
Carbon Tetrahedral
Builder
G1:M1:V1 - New
Viewer
Build
Select Placement

Mouse Button	Action	Function
Left	Click	Selects or inserts item
	Drag Left/Right	Rotates about Y-axis
	Drag Up/Down	Rotates about X-axis
Center/Left-Right	Drag	Translation of molecule
Right	Drag Left/Right	Rotates about Z-axis
	Drag Up/Down	Zooms in and out
Note: Holding down the Tab key limits mouse action to the closest distinct fragment.		

Molecule Building

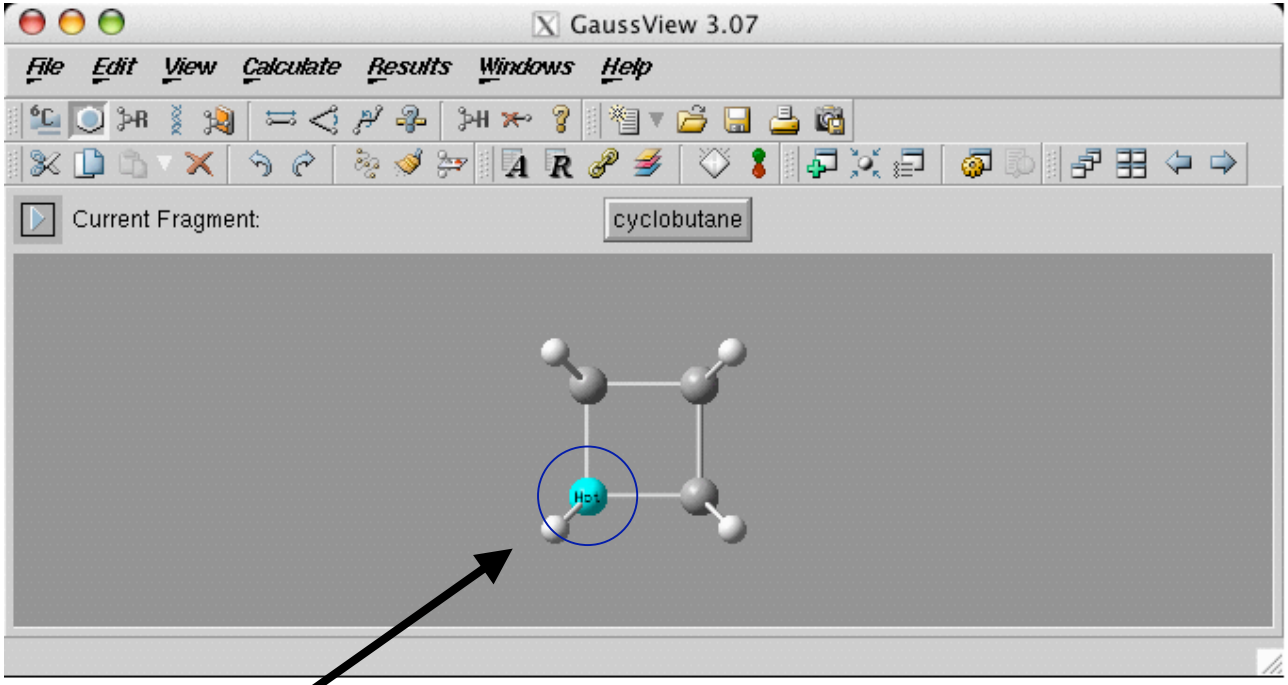
Selected fragments
Are previewed here

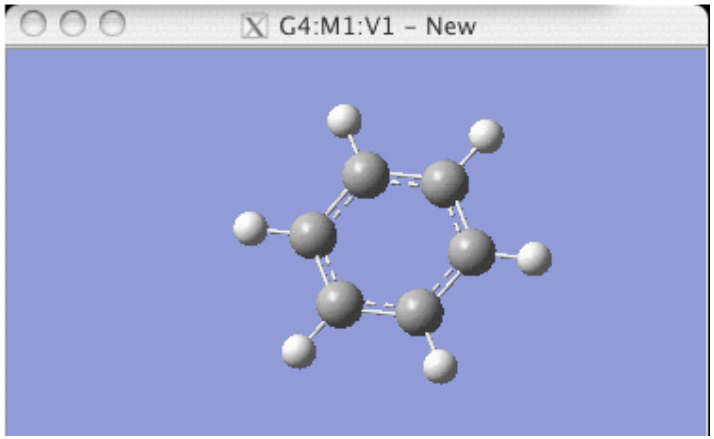
Fragments are
Selected



Molecule is put together
Here

Molecule Building

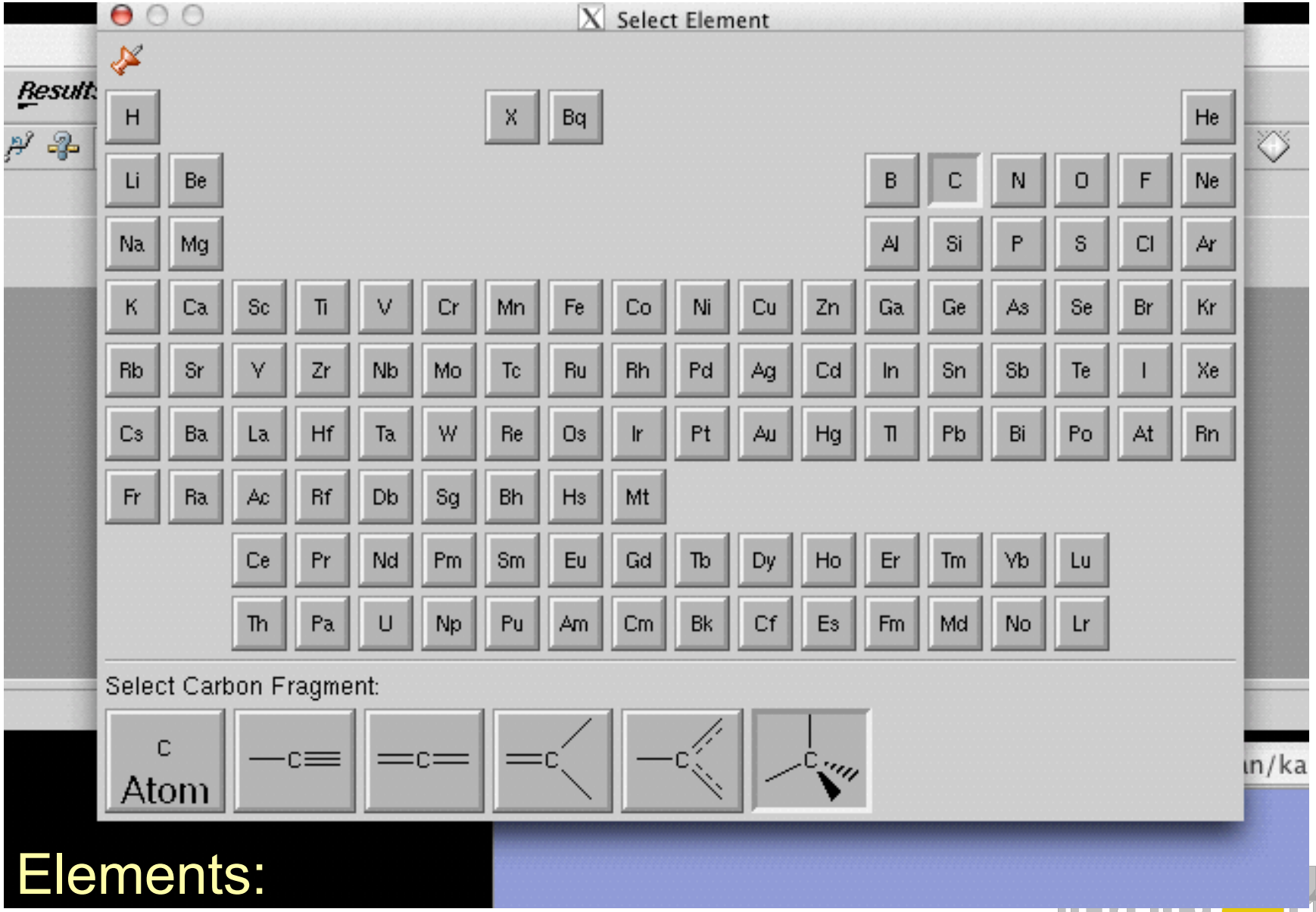




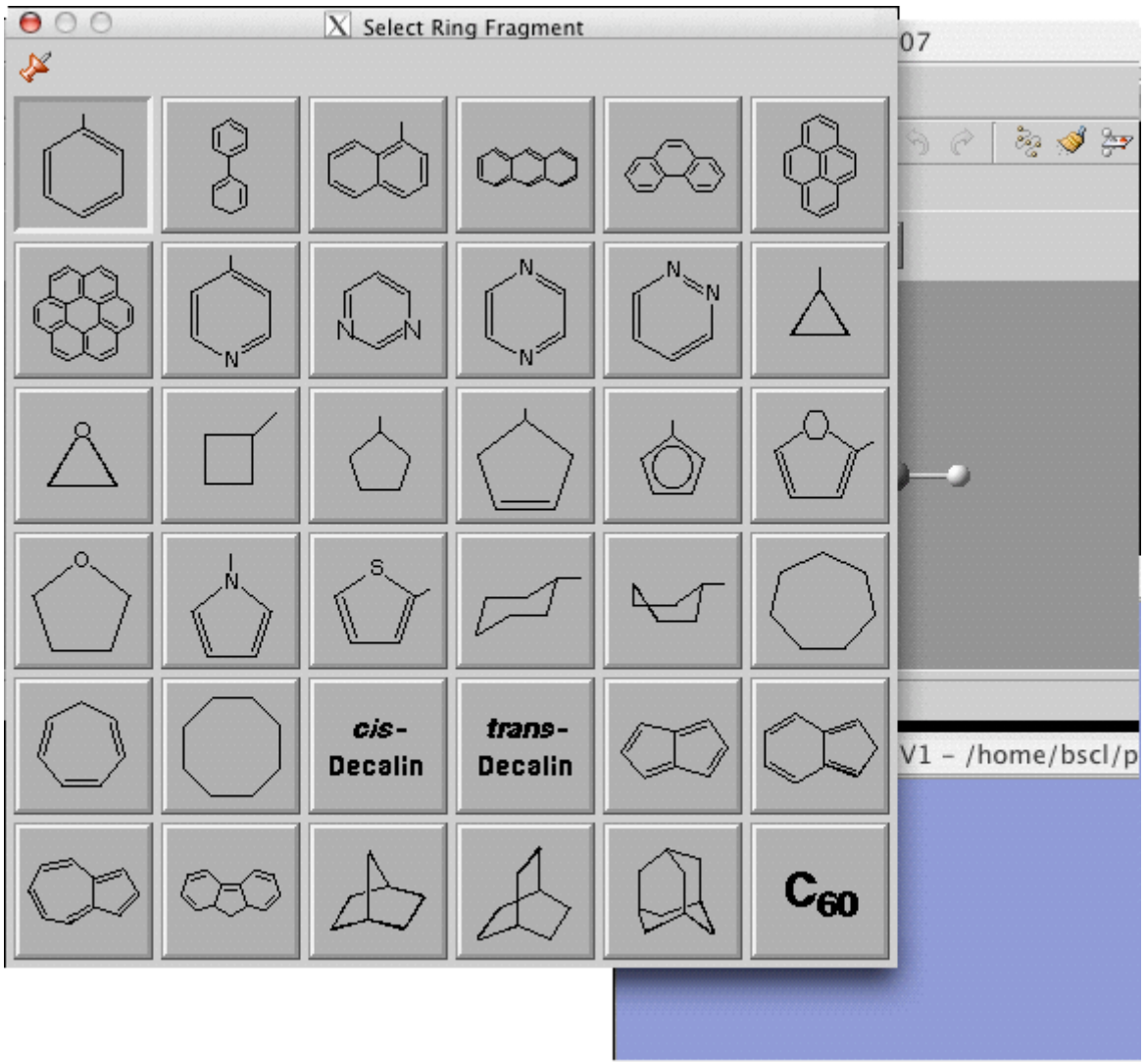
The atom labeled "Hot" is is where the fragment will attach to the system you are building.

Steps to Building

- Choose an atom or fragment
- Choose the location of the fragment that will attach to your molecule in the builder window
- Select/add the fragment to your molecule in the viewer window
- repeat


Select Element
H
X
Bq
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Cs
Ba
La
Hf
Ta
W
Re
Os
Ir
Pt
Au
Hg
Tl
Pb
Bi
Po
At
Rn
Fr
Ra
Ac
Rf
Db
Sg
Bh
Hs
Mt
Ce
Pr
Nd
Pm
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu
Th
Pa
U
Np
Pu
Am
Cm
Bk
Cf
Es
Fm
Md
No
Lr
Select Carbon Fragment:
C
Atom

Elements:



Ring Fragments:

Description • Input • Submit • Visualize

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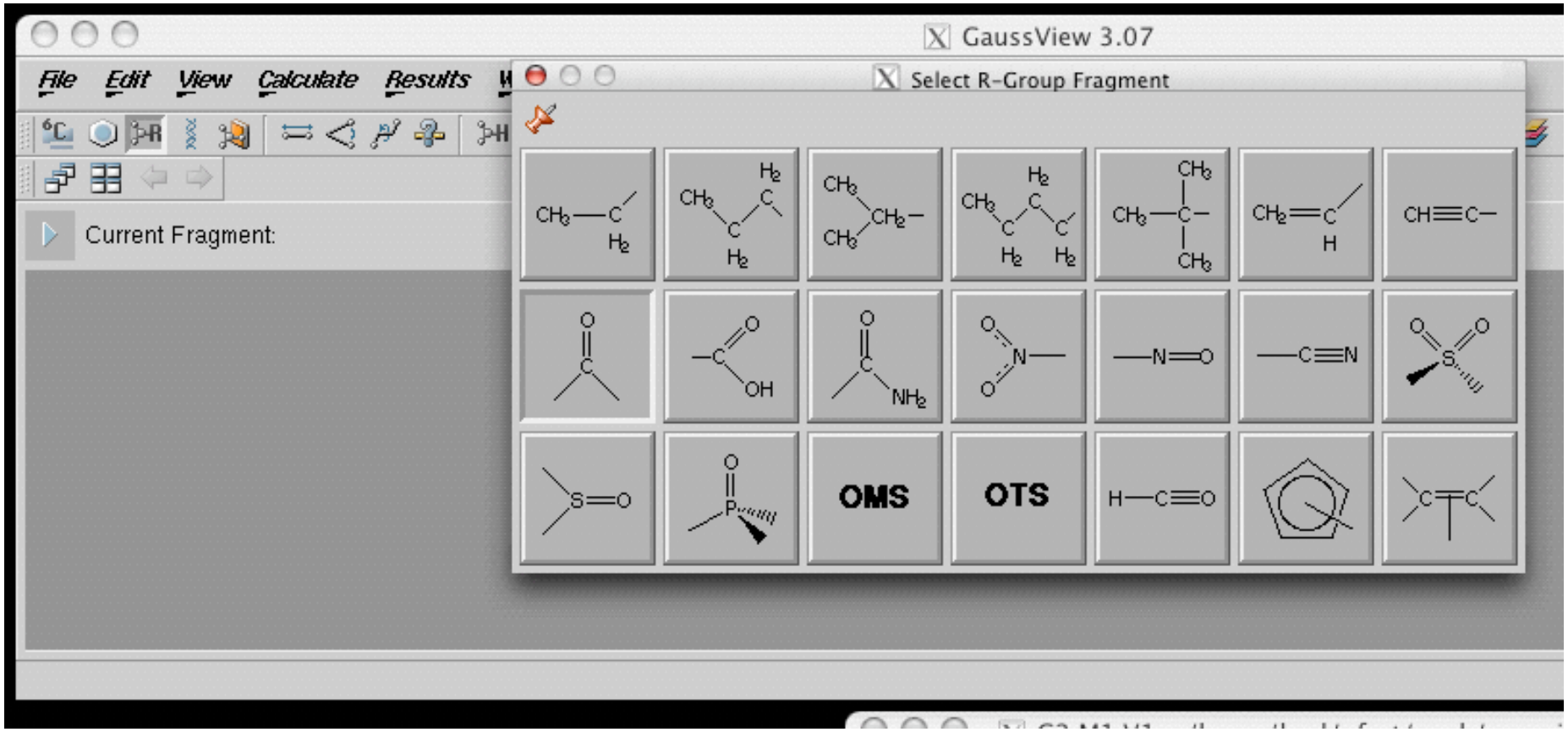
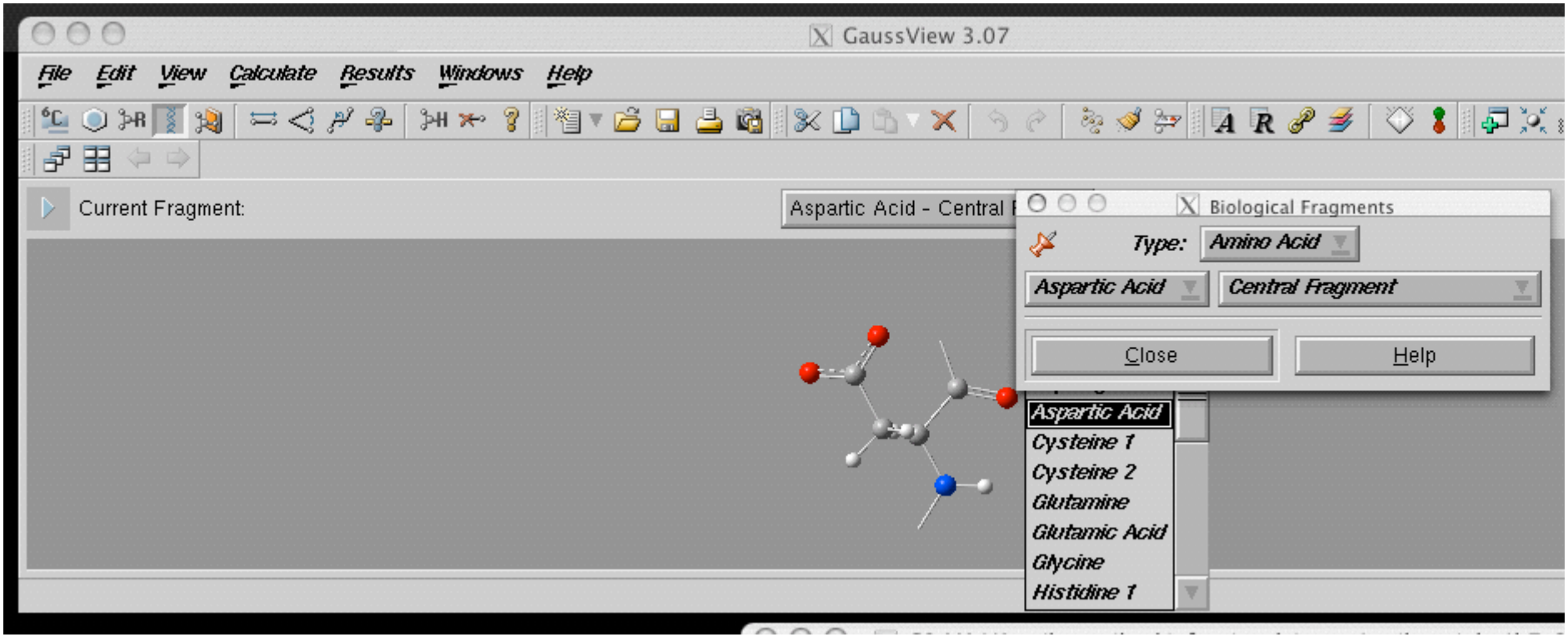
R-Group Fragments:



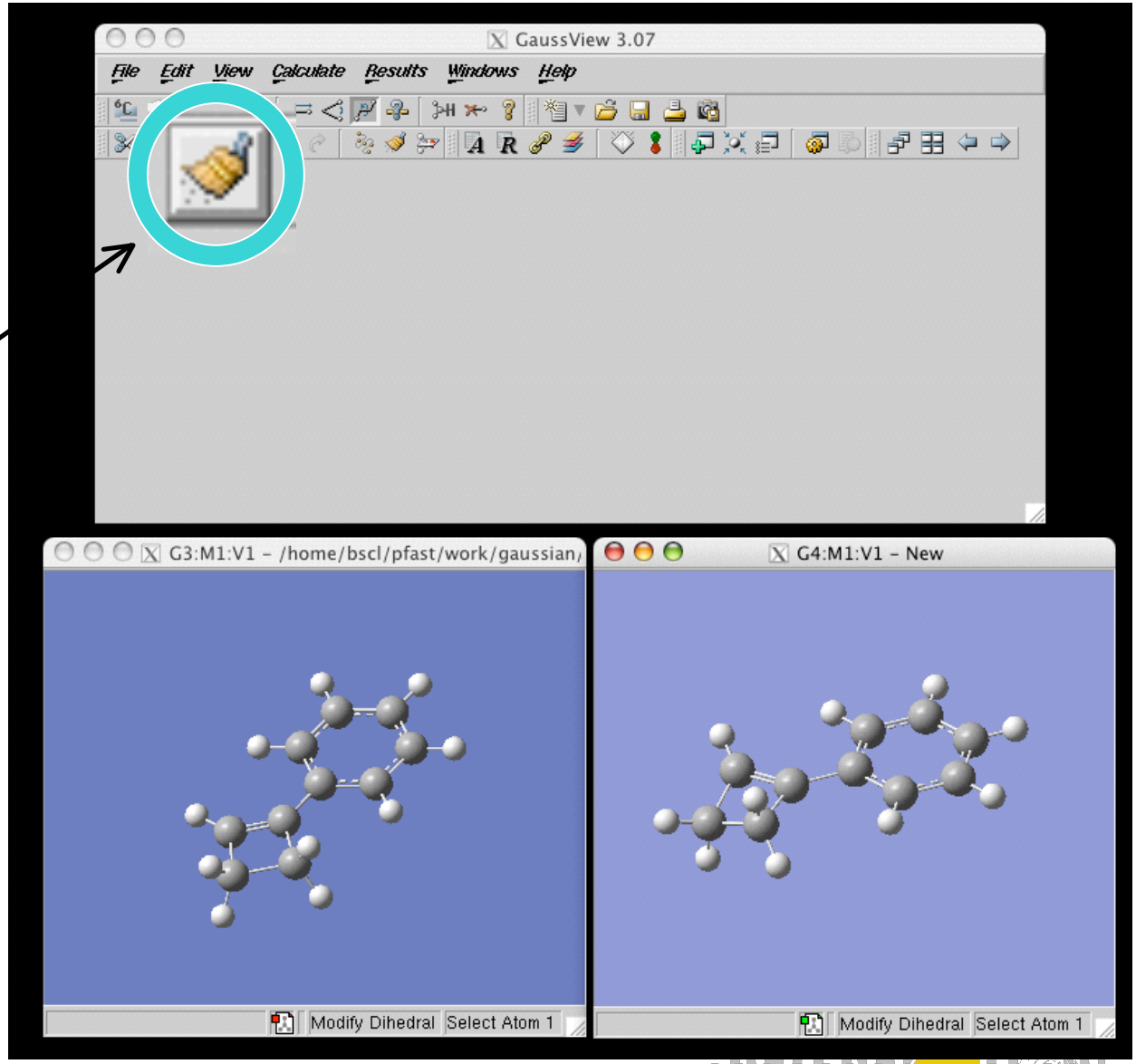
Biological Fragments:



Molecule Building

clean up

This option will use a MM calculation to optimize the geometry (very fast).



Submitting Calculations

Interactive:

Command:

```
g03 < input_file > output_file
```

Notes:

1) **input and output files can use absolute or relative pathnames**
2) **Gaussian temporary files can be redirected by setting the GAUSS_SCRDIR environment variable.**

```
setenv GAUSS_SCRDIR /scratch/pfast
```

3) **BE CAREFUL how long you run interactively**

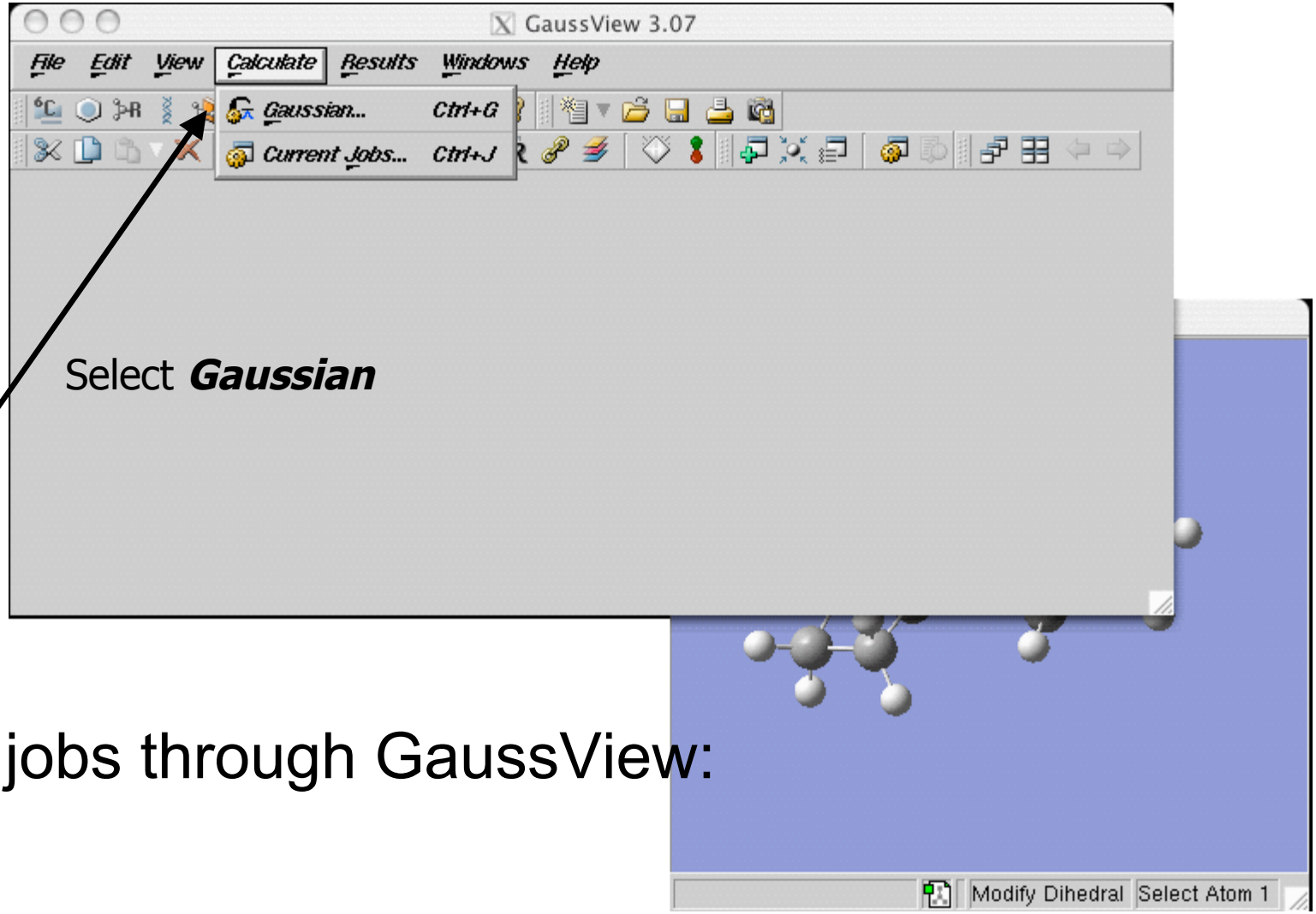
Batch:

Command:

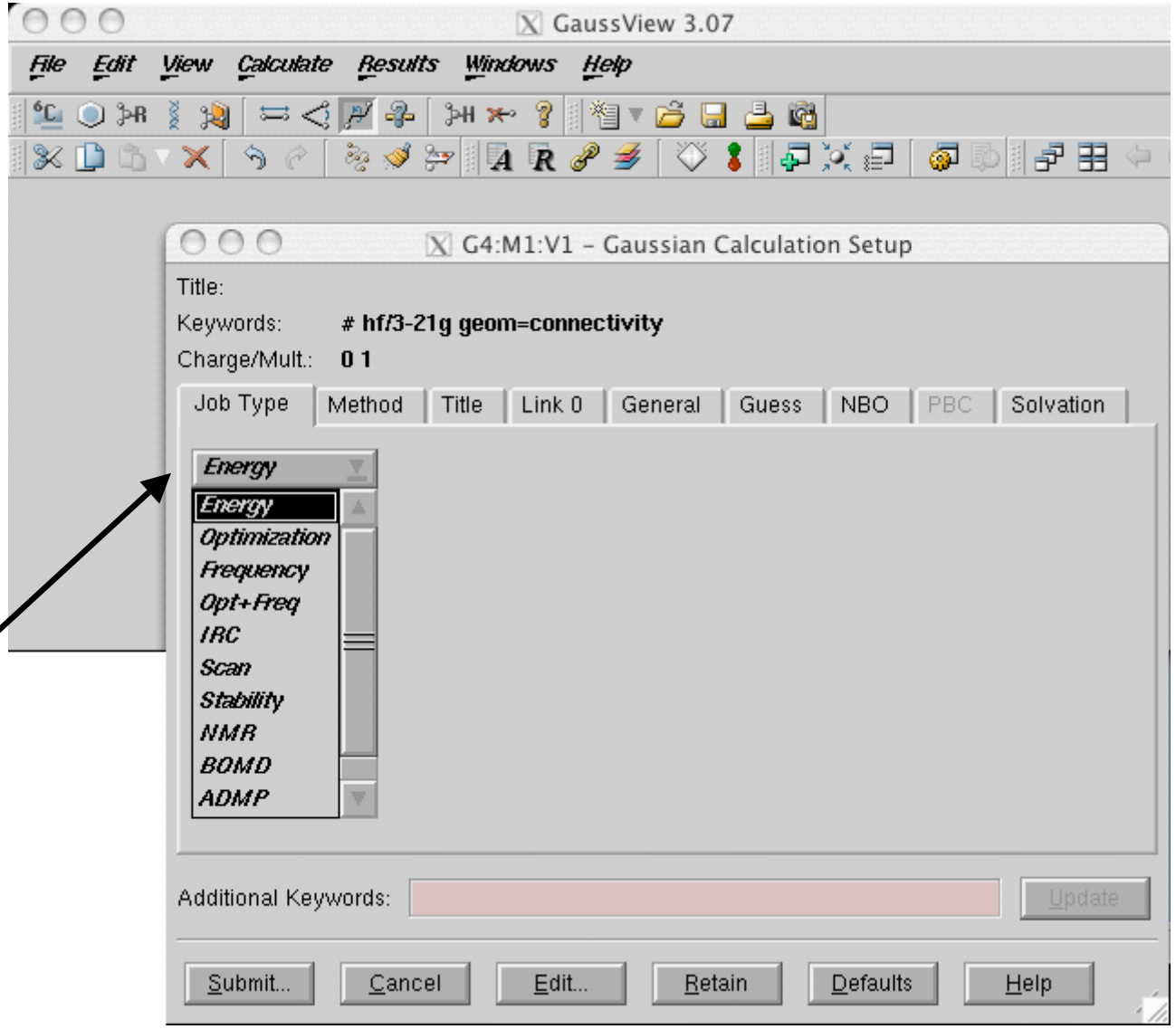
qg03 [-options] input_file

Options:

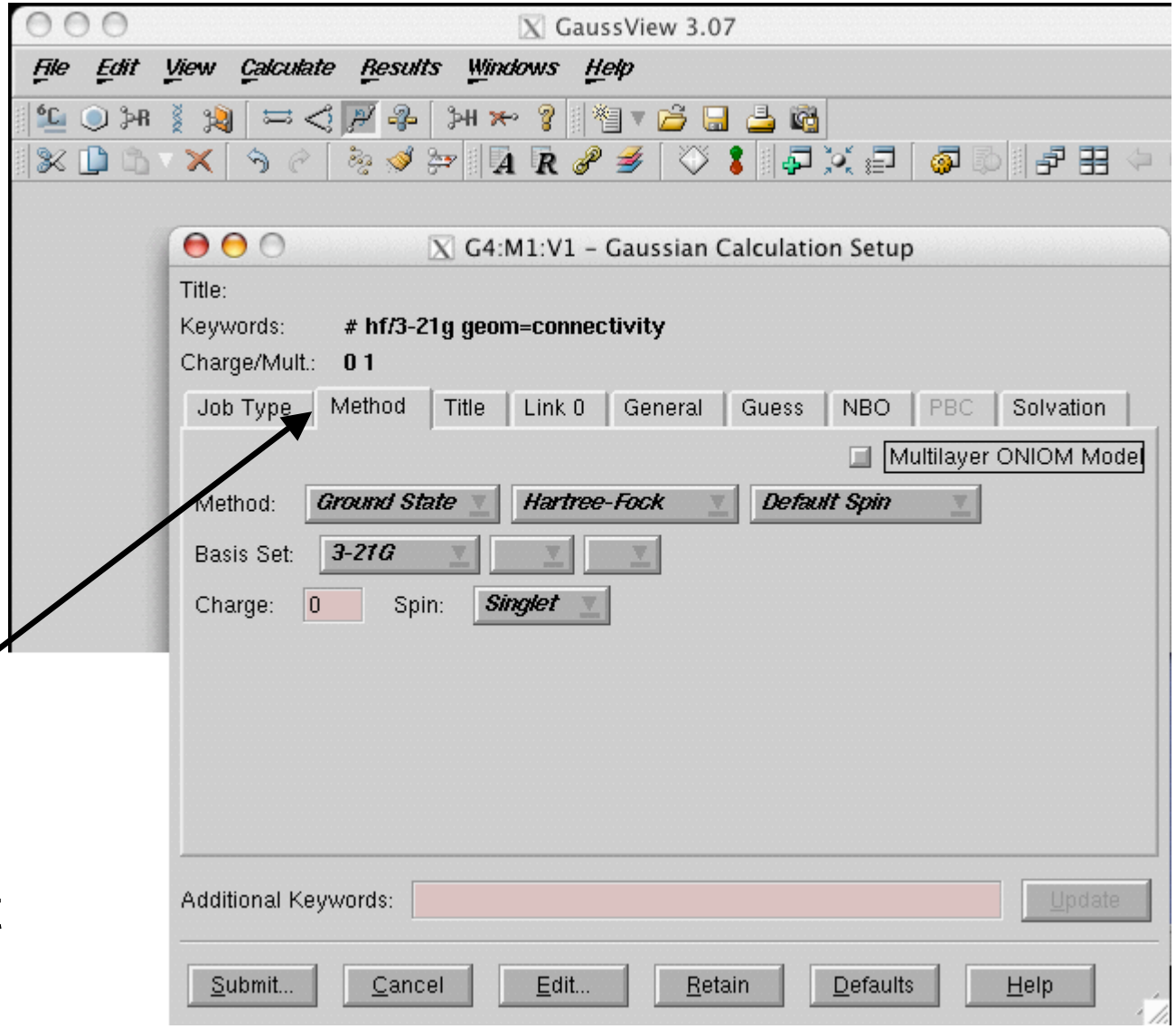
-h	help, display a usage list and the defaults
-e	email notification
-m	total amount of memory
-n	node, choose the particular processor
-p	number of processors
-r	run?
-s	scratch space
-t	amount of wallclock time



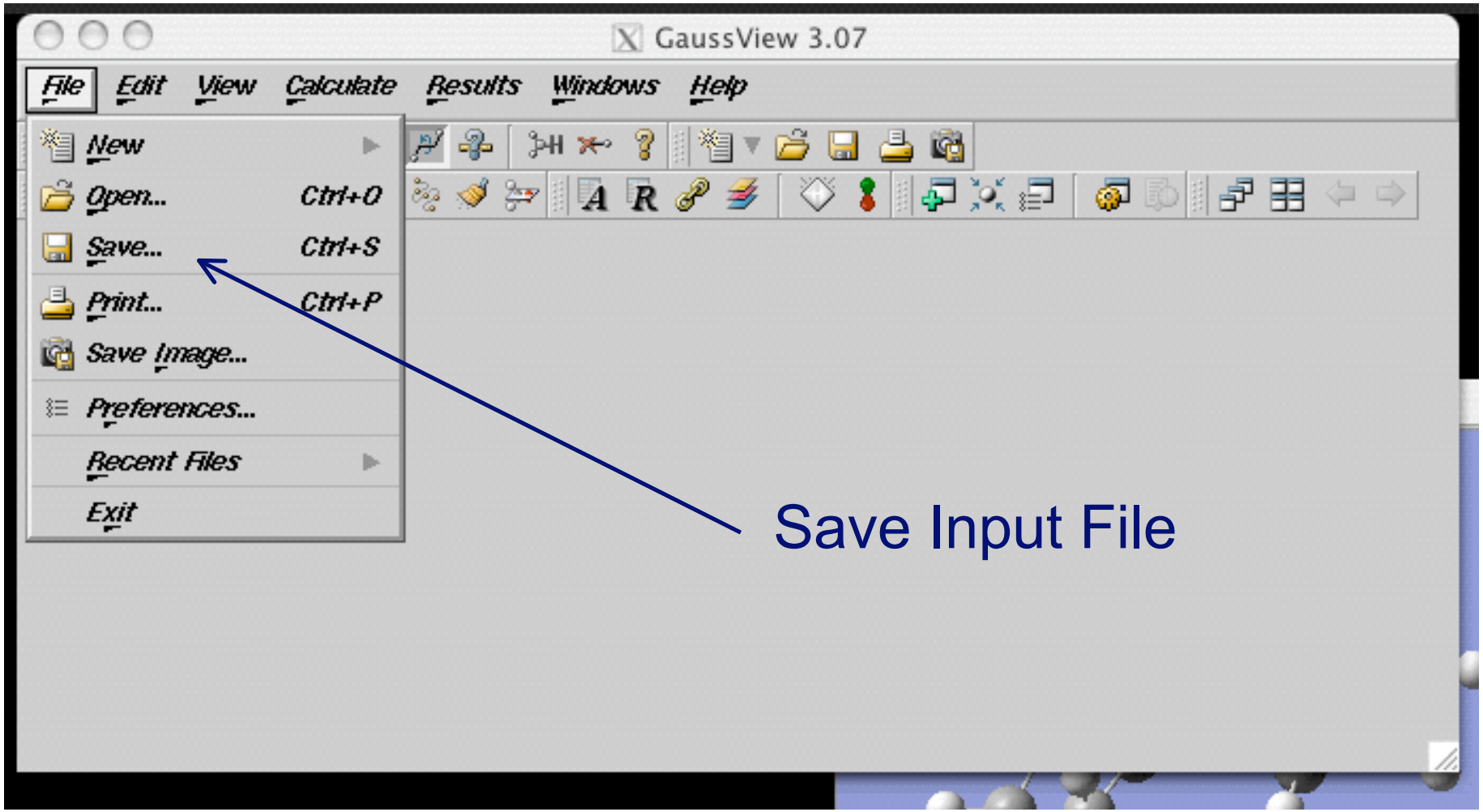
Submitting jobs through GaussView:

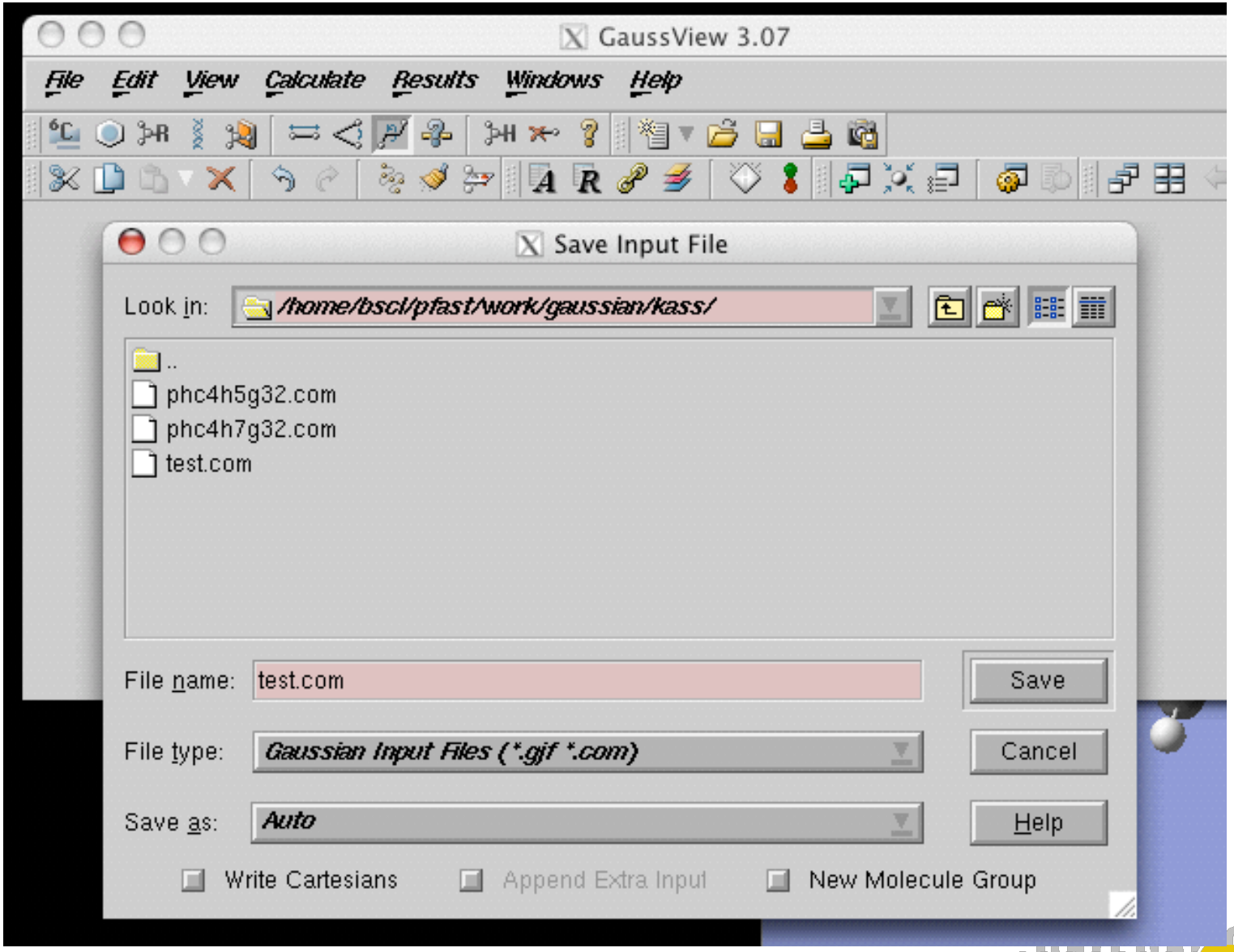


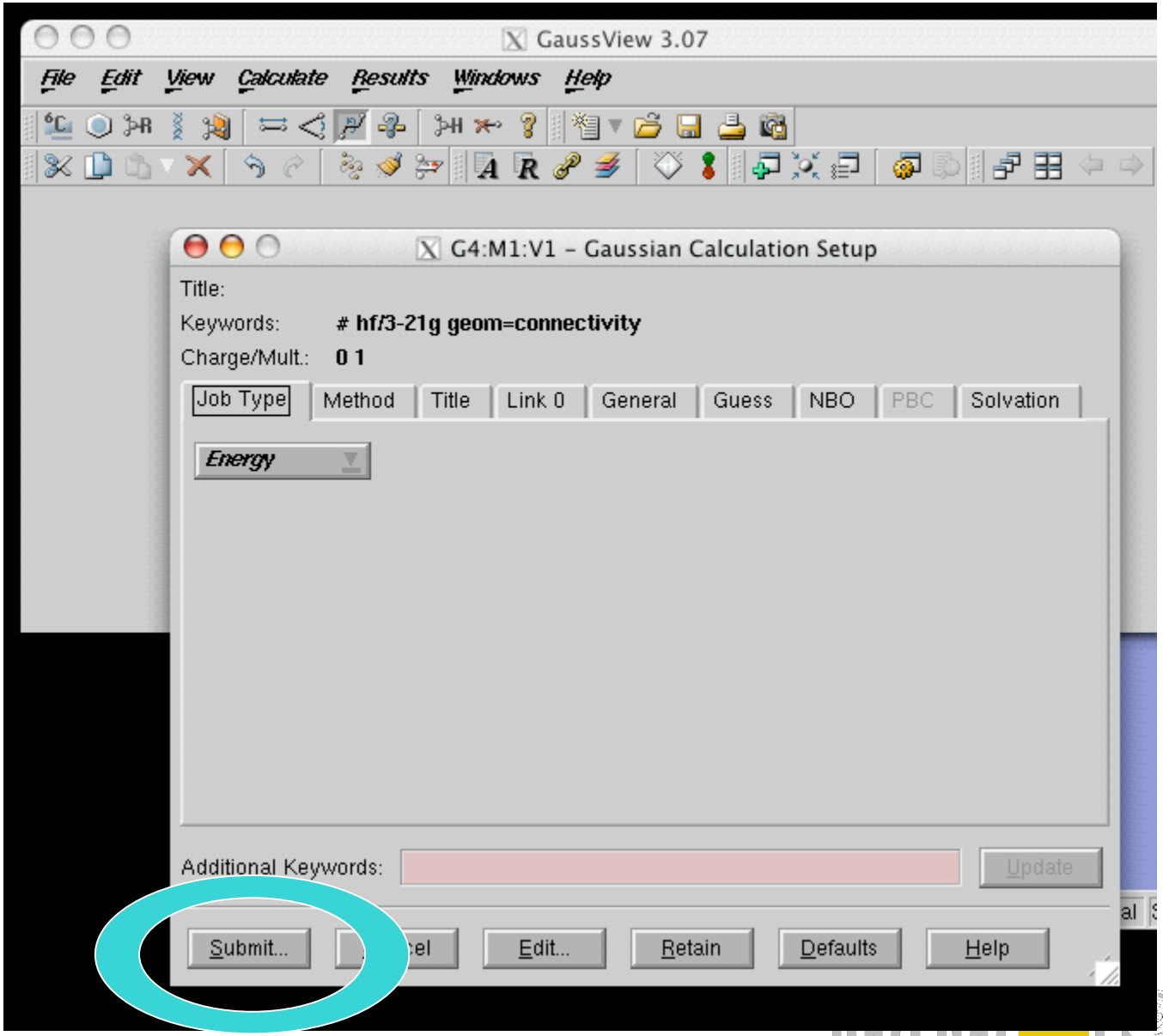
Choose Job Type

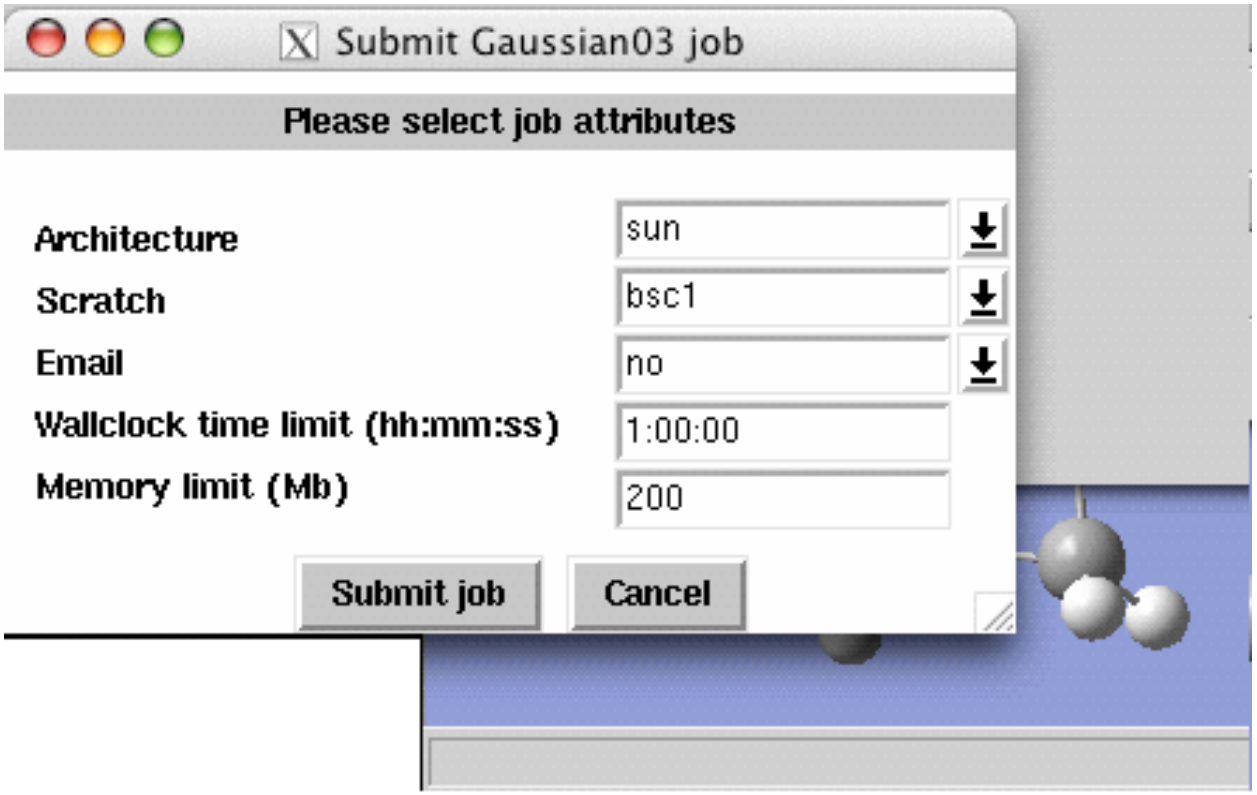


Method & Basis Set


GaussView 3.07
File
Edit
View
Calculate
Results
Windows
Help
New
Open... Ctrl+O
Save... Ctrl+S
Print... Ctrl+P
Save Image...
Preferences...
Recent Files
Exit
Save Input File


GaussView 3.07
File Edit View Calculate Results Windows Help
Save Input File
Look in: /home/bscl/pfast/work/gaussian/kass/
..
phc4h5g32.com
phc4h7g32.com
test.com
File name: test.com
Save
File type: Gaussian Input Files (*.gjf *.com)
Cancel
Save as: Auto
Help
Write Cartesians
Append Extra Input
New Molecule Group


GaussView 3.07
File Edit View Calculate Results Windows Help
G4:M1:V1 - Gaussian Calculation Setup
Title:
Keywords: # hf/3-21g geom=connectivity
Charge/Mult.: 0 1
Job Type Method Title Link 0 General Guess NBO PBC Solvation
Energy
Additional Keywords:
Update
Submit...
Edit...
Retain
Defaults
Help



The submission dialogue box will appear a little different depending on which machine you are running GaussView on.

Submitting your Gaussian job

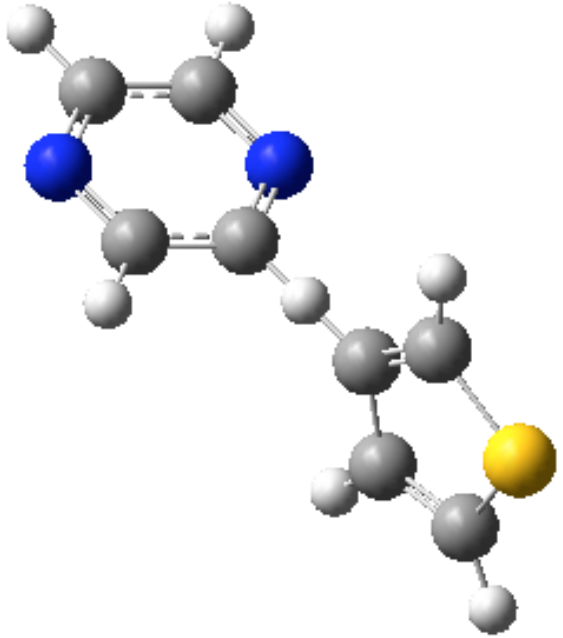
If you haven't saved your input file yet, Gaussview will Prompt you to save your input file.

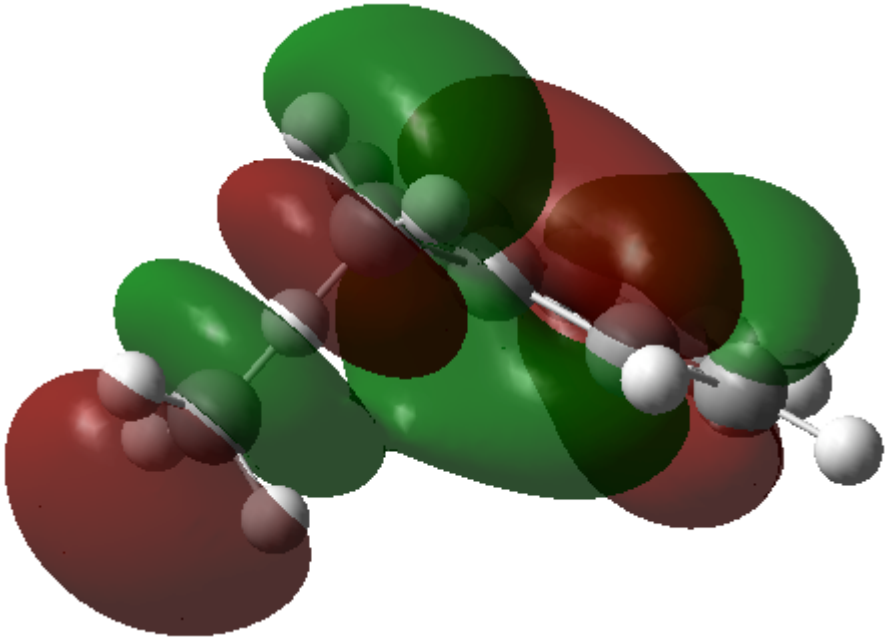
You will name the input file, and then submit the calculation.

When Gaussian is finished running, you will receive a message in Gaussview.

How to Visualize

Visualization Features





Description • Input • Submit • Visualize

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How to view your output

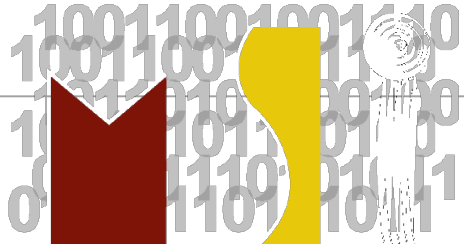
- Your submitted calculation will run in the background.
- When it is complete, Gaussview will inform you and ask you if you wish to view an output file.
- From the list of files, you can pick your output (something.chk)

How to view your output

- If you ever want to open an output file again, you can go to:

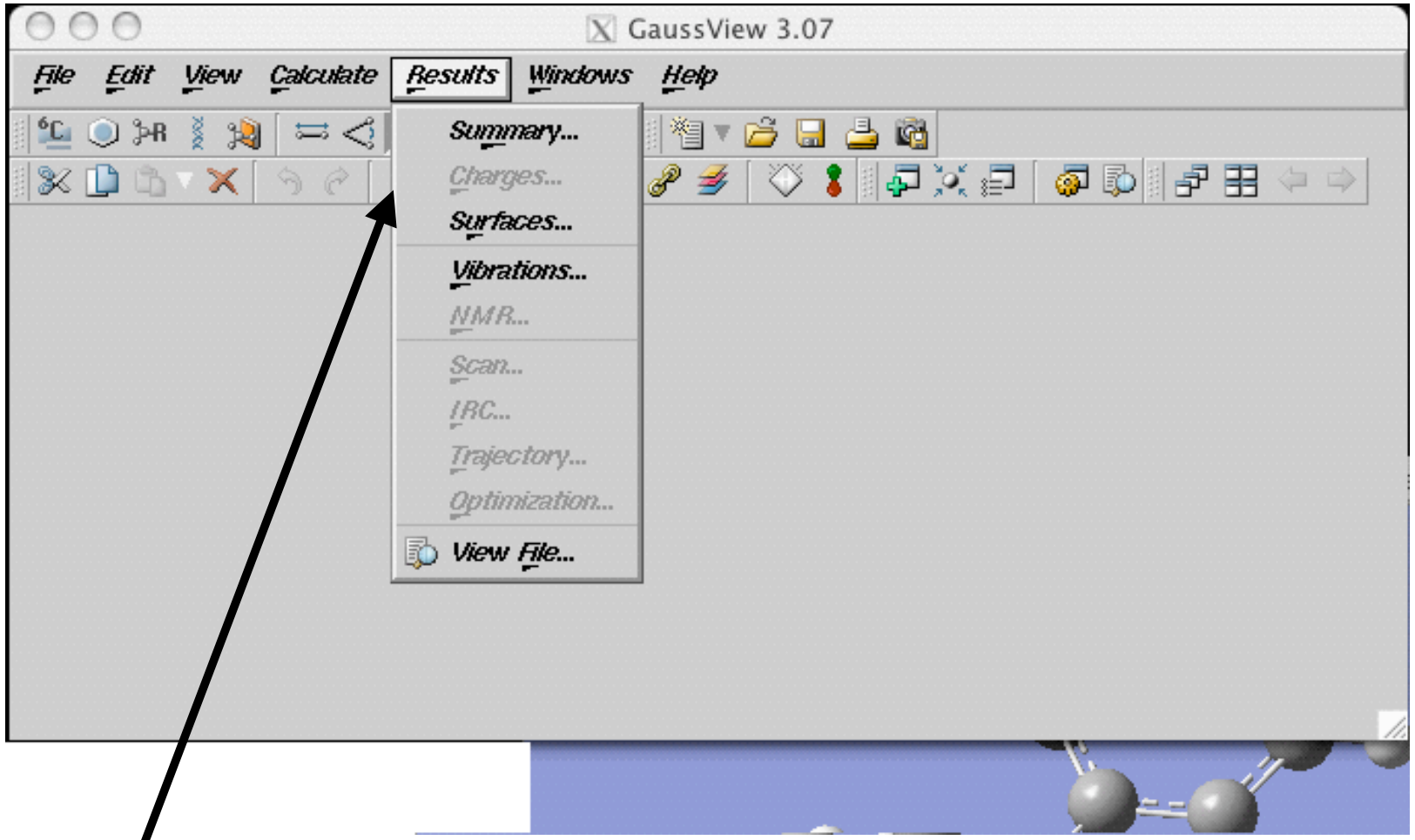
  File → Open

  In the GaussView menus to open any output file.

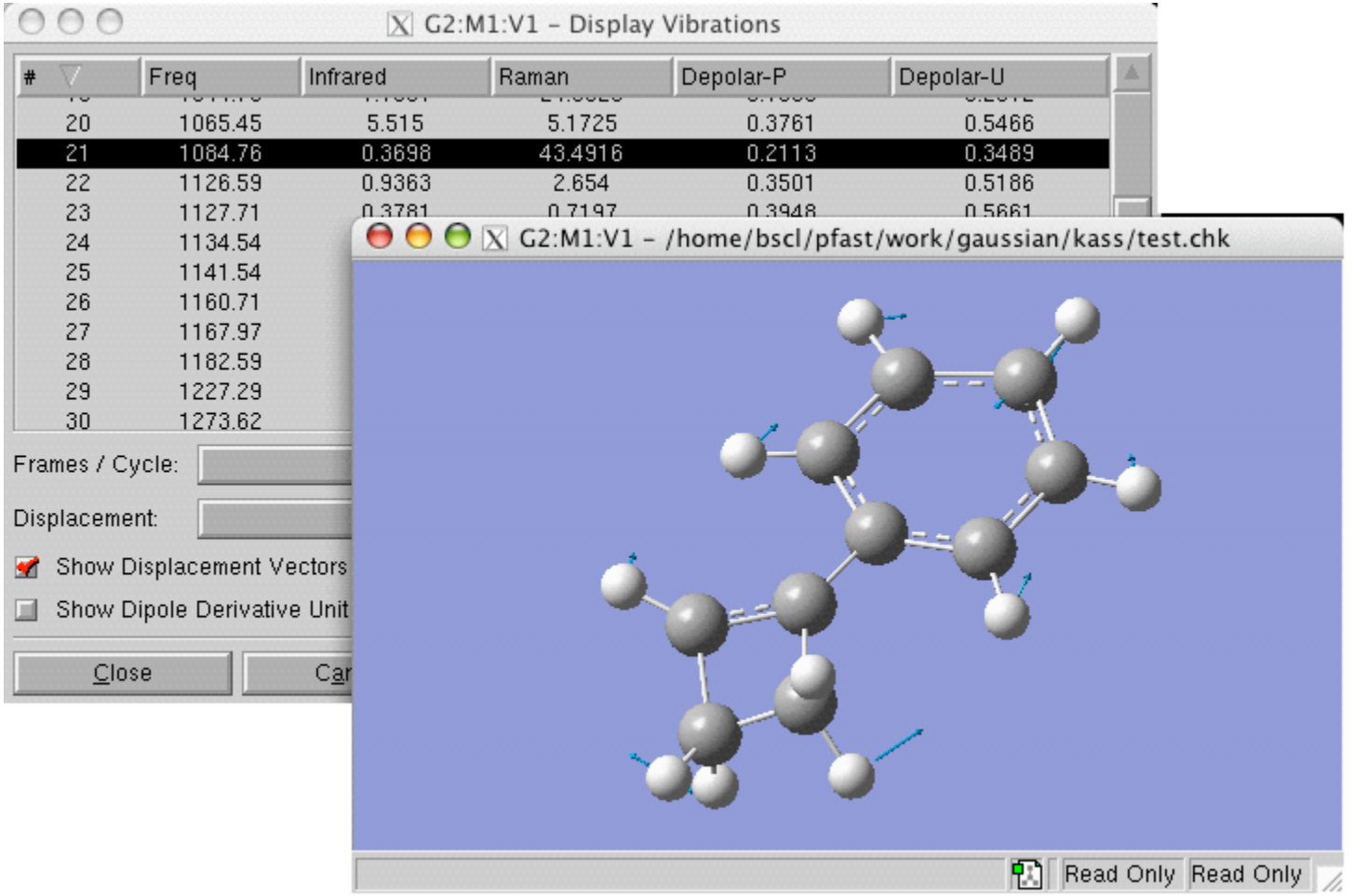


Output that can be visualized

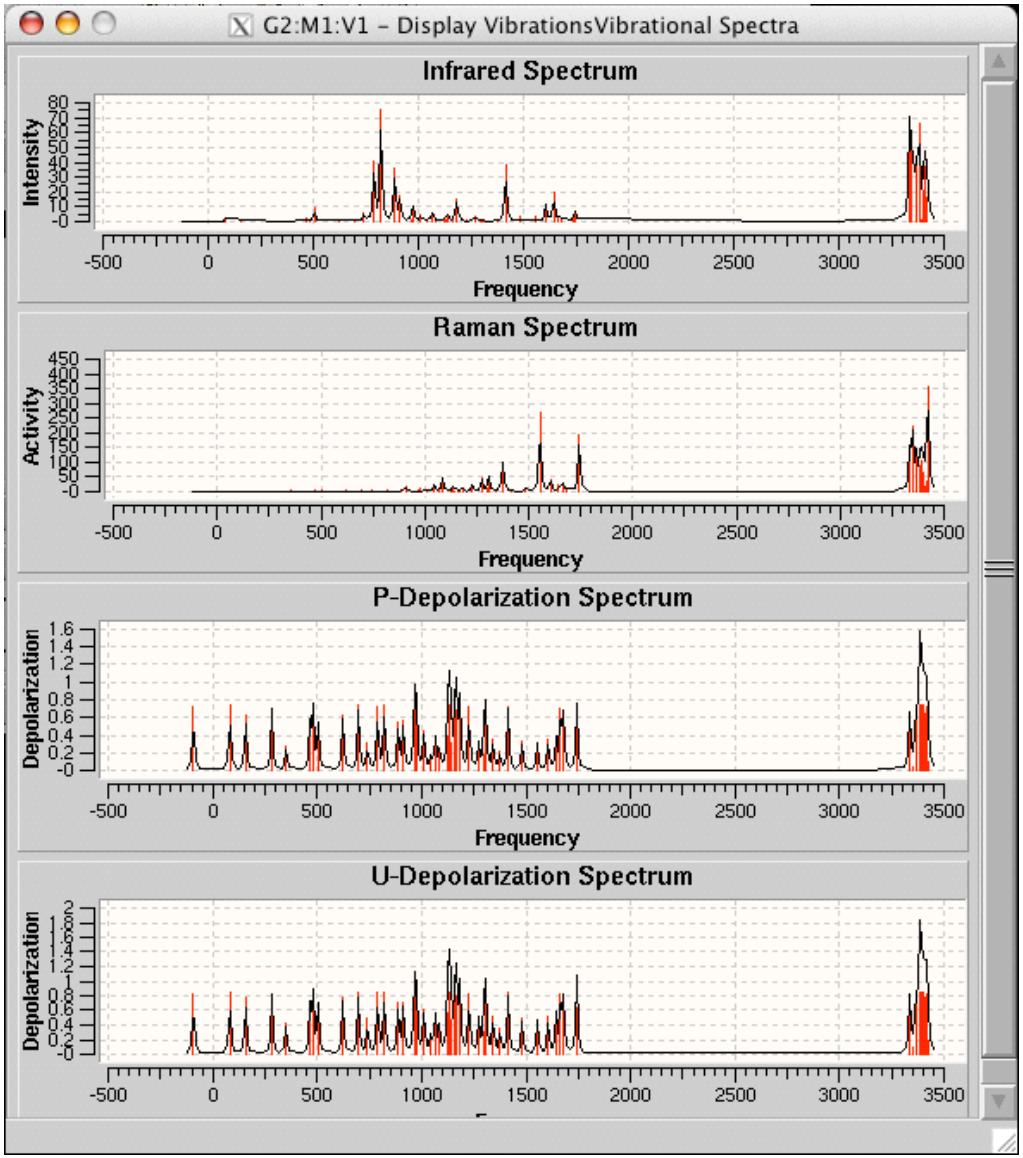
- Geometry
- Vibrations
- Orbitals
- Electron density
- Electrostatic potential



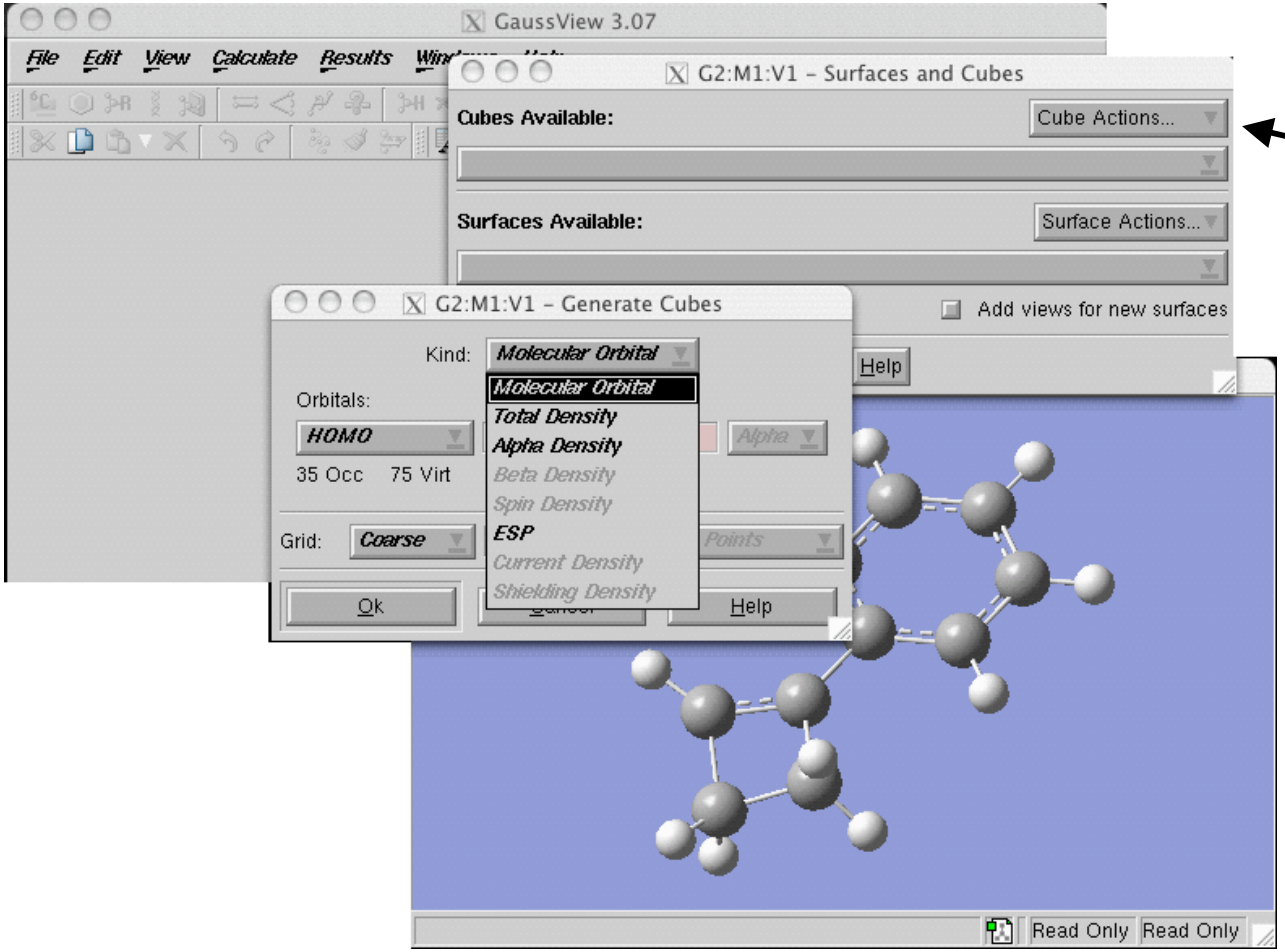
Main results menu



Frequencies

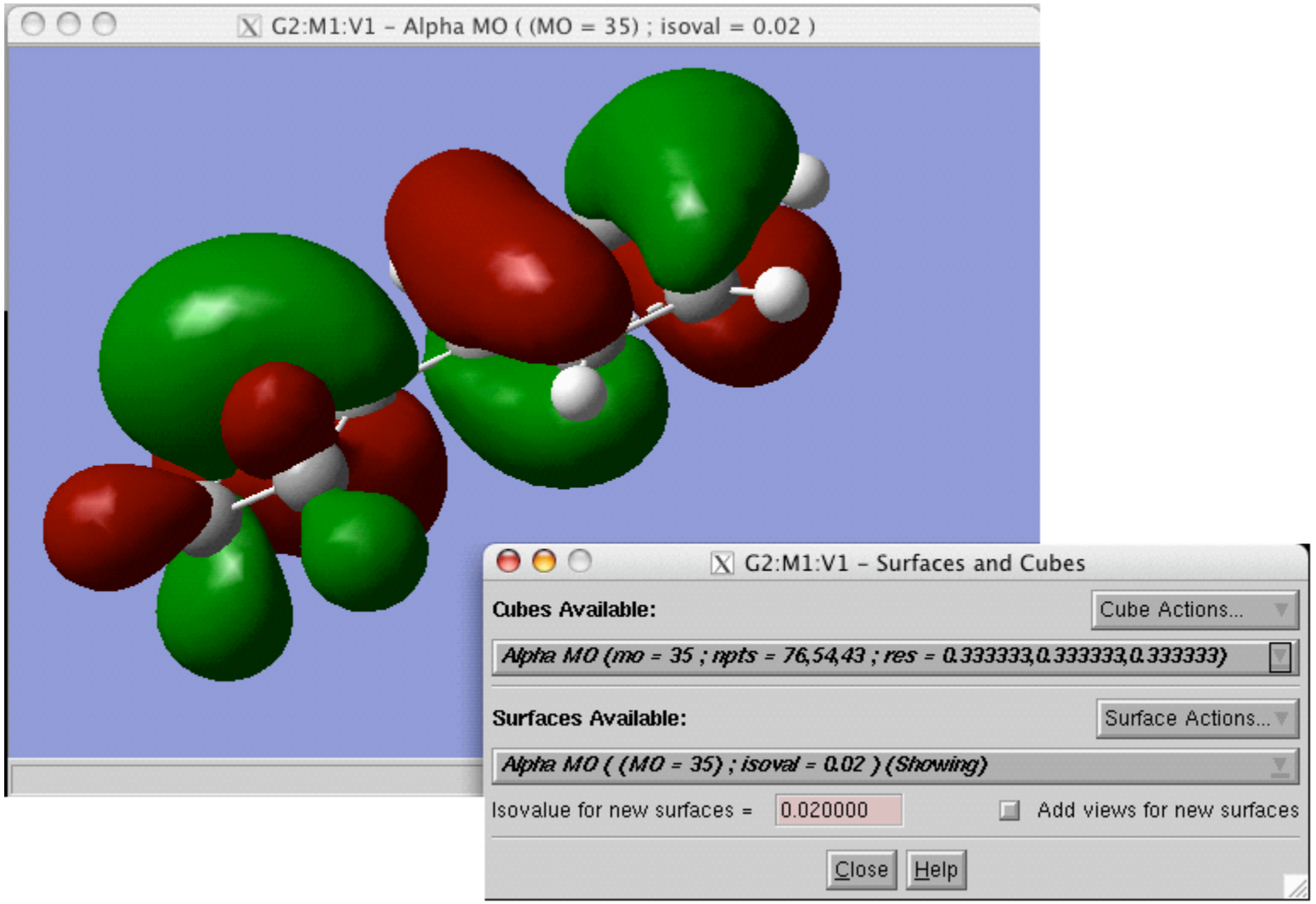

G2:M1:V1 - Display VibrationsVibrational Spectra
Infrared Spectrum
Intensity
Frequency
Raman Spectrum
Activity
Frequency
P-Depolarization Spectrum
Depolarization
Frequency
U-Depolarization Spectrum
Depolarization

Spectra



A cube file is a format of 3-D data that can be plotted.

You can generate a cube file to display orbitals, electron densities, electrostatic potentials, etc.



Description • Input • Submit • Visualize

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Questions?

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