Background

Some background from the Gaussian web site:

http://www.gaussian.com/

GaussView5 links:

https://www.d.umn.edu/~psiders/courses/chem5650/gaussviewtutorial/tutorial.html

https://www.mtholyoke.edu/courses/jwijngaa/PS/Gaussview2.pdf

Principles

1. **Variation Principle**

$$\int \Psi_{approx} * H \Psi_{approx} dV = E_{approx} \geq E_{\text{exact ground state}}$$

The Hamiltonian is always “exact”

The wavefunction is always approximate, and is **varied** to reach the lowest possible ground state energy with the type of function **chosen**

More exact if:

1)Larger, more detailed **basis set** of atomic orbitals

2)More electron-electron **correlation (dodging)**

Specific Objectives:

1. Create an input file for water. Compute its equilibrium energy and structure, and examine its molecular orbitals.

2. Compute the geometry and energy of a pair of H-bonded waters.

3. Compute and compare vibrational frequencies for N_2O, and CO_2 at different levels of accuracy and make assignments to observed spectra.

4. Create and examine benzene MOs and vibrations, including benzene-d1.

GaussView lets you examine the results of Gaussian calculations using a variety of graphical techniques.

Gaussian results that can be viewed graphically include the following:

❖❖ **Optimized molecular structures**.
❖❖ **Molecular orbitals.**
❖❖ Electron density surfaces from any computed density.
❖❖ Electrostatic potential surfaces.
❖❖ Surfaces for magnetic properties.
❖❖ Surfaces may also be viewed as contours.
❖❖ **Atomic charges and dipole moments**.
❖❖ **Animation of the normal modes corresponding to vibrational frequencies.**
❖❖ IR, Raman, NMR, VCD and other spectra.
❖❖ Molecular stereochemistry information.
❖❖ Animation of geometry optimizations, IRC reaction path following, potential energy surface scans, and
ADMP and BOMD trajectories. Two variable scans can also be displayed as 3D plots.
❖❖ Plots of the total energy and other data from the same job types as in the previous item.

Outline

1. *wiki.crc.nd.edu/wiki/images/d/d7/Gaussview-5-ref.pdf*
2. Login with netid, password
3. find a work directory **c:\users\your netid**
   and go to it
4. find the GaussView icon under **All programs GaussView 5.0 icon**
   open
   click help --- just to see what is there, including **tutorials**
5. File ->Preferences : choose: launch directory
   notice Display format
   find the **Gaussian 09W icon** and open it
   File-> Preferences: choose: launch directory
6. Look at *Gaussview-5-ref.pdf*
   what can be done
   typographic conventions

Menu items = blue
Buttons =green
Dialog names = Black. Gaussian
keywords and options like Opt=QST2 = Purple

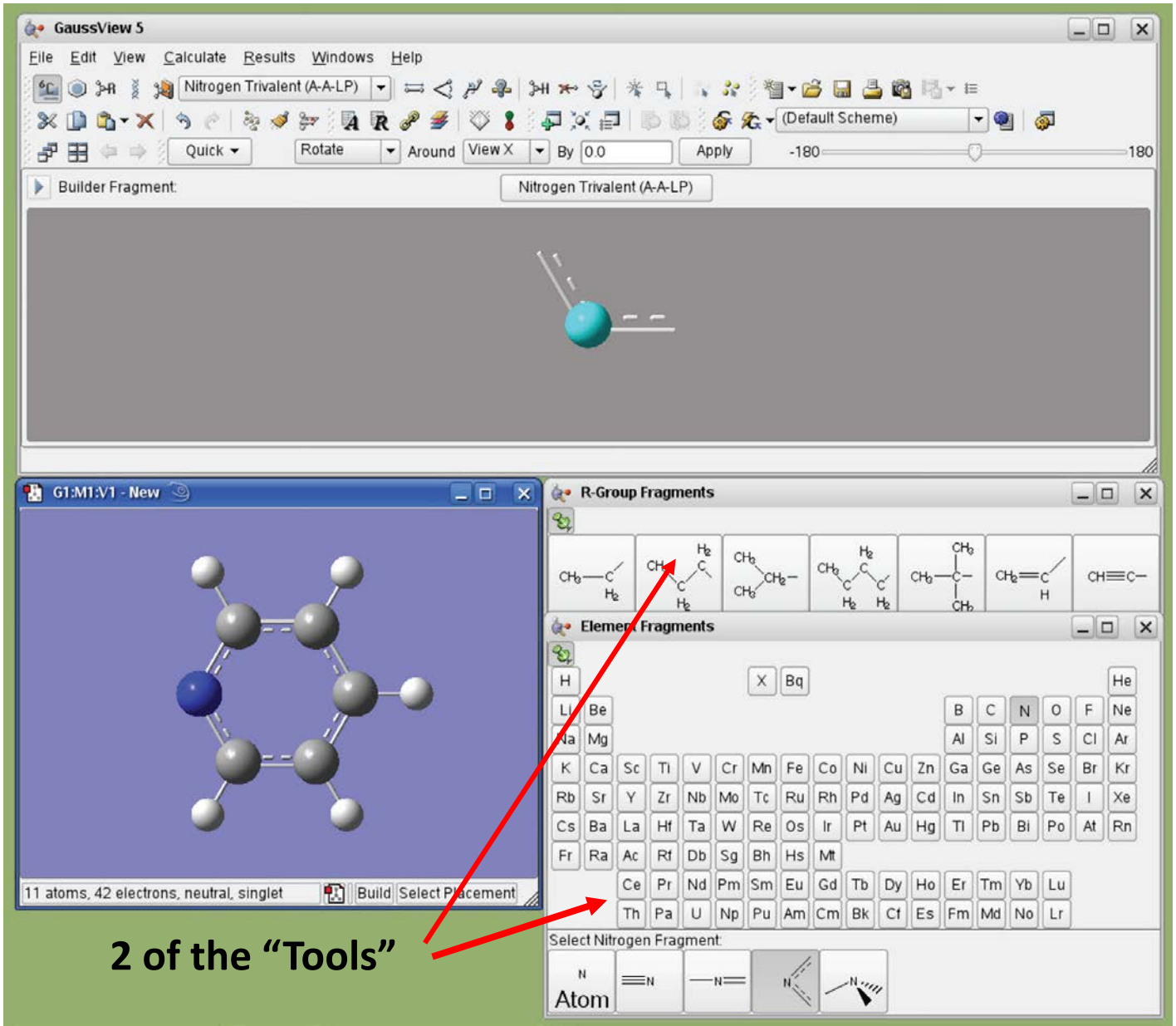
7. Main Interface Control Panel
Current fragment
Various Tool Bars (detachable, moveable
View windows
Dialogs
Preferences

Main Interface: Control Panel

Tool Bars

Current Fragment

a View Window



Hovering the MOUSE over an icon will tell its function

in the lower left corner of screen

Outline -2

Tool bars and Icons
  hovering over icon & look lower left

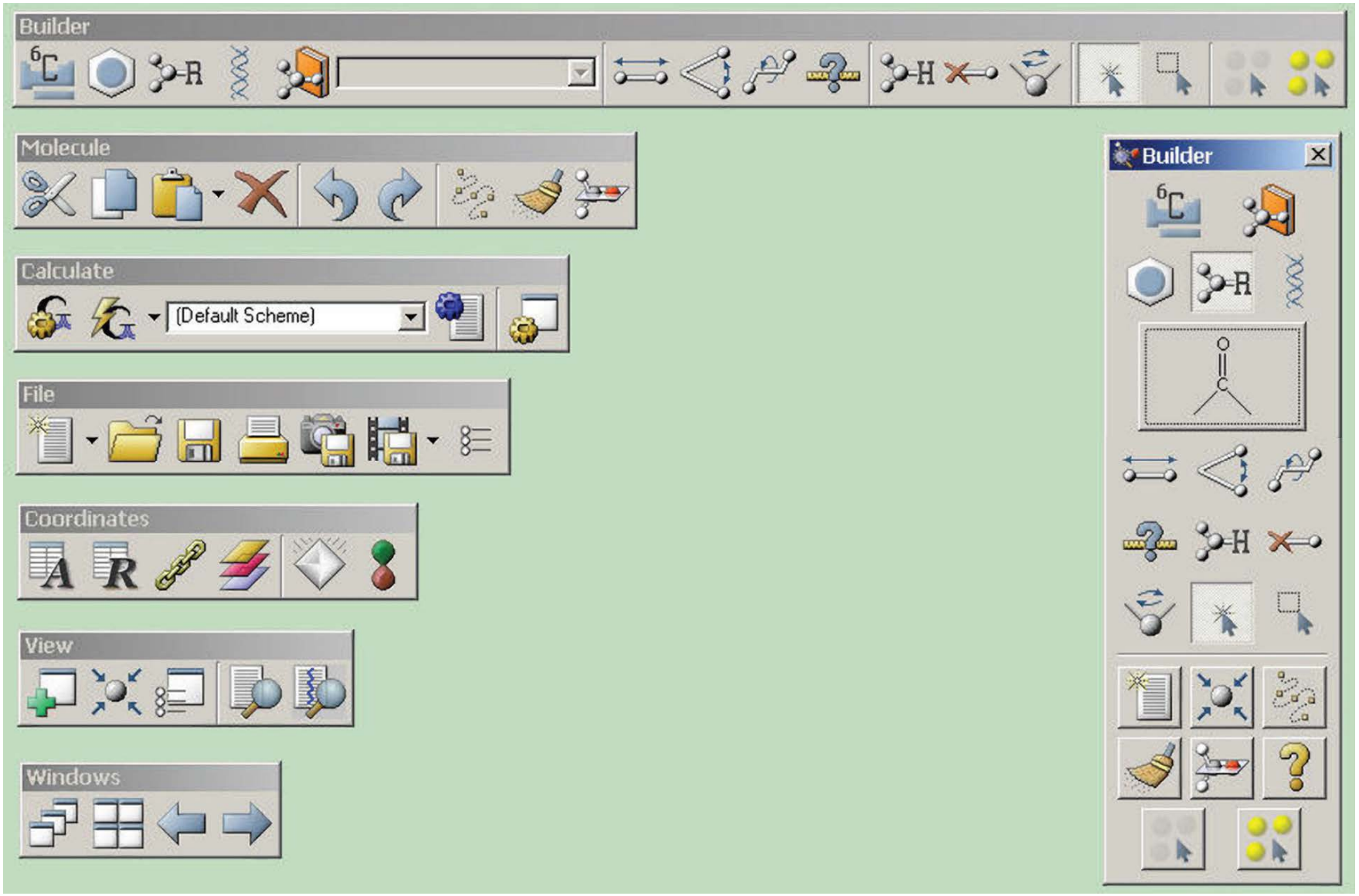
8. View Builder
    5 items for creating “molecules”

 UNDO = contrl-z
REDO = contrl-y

 Positioning
  bond length
  angle
 dihedral
    options to know about
 inquire
 add valence
 delete atom
  selecting

clean
symmetrize

All of the Tool Bars:



5 tools for constructing a molecule

get forms any element by clicking on any atom

pick one of an assortment of rings

pick one of an assortment common small groups

protein and nucleic acid components

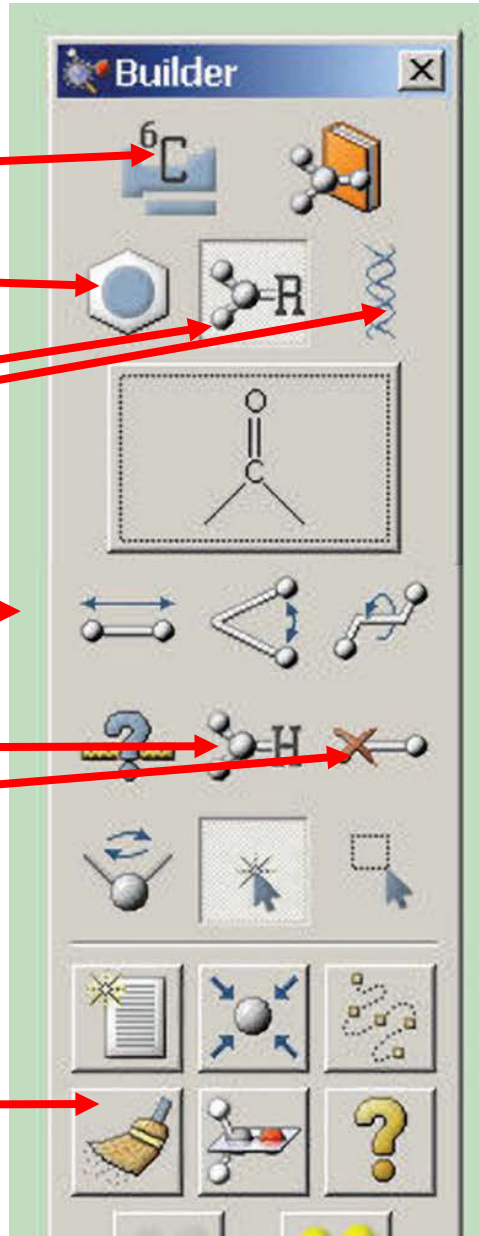
measuring and changing:

bond lengths, angles, and dihedrals

Add a valence (H atom):

delete an atom:

“Clean”: will roughly optimize the structure you have made



UNDO = control-z

REDO = control-y

Specific Objectives:

1. Create an input file for water. Compute its equilibrium energy and structure, and examine its molecular orbitals.

2. Compute the geometry and energy of a pair of H-bonded waters.

3. Compute and compare vibrational frequencies for N_2O, and CO_2 at different levels of accuracy and make assignments to observed spectra.

4. Create and examine benzene MOs and vibrations, including benzene-d1.

The essential ingredients of this file come in the following order: the ***route section*** **(or "route card")** begins with #, and contains the method/basis (e.g., hf/6-31g) and other key words (separated by any number of spaces, in any order, case insensitive (non-ambiguous abbreviations are allowed). The route section may contain any number of lines, terminated by a blank line.

Example input file for H_2O: h2o-1.gjf

```
%chk=mydirectory/h2o-1.chk
# hf/3-21g  opt pop=full

Title info

0 1
o   0.   0.    0.
h   1.   0.   0.
h   0.   1.    0.

```

blank lines mark the different sections of input

Next is the ***net charge and multiplicity***. (multiplicity = degeneracy of the total electron spin state = 2S + 1. Total **ANY** angular momentum squared = $S(S+1)(h/2\pi)^2$. For a singlet state (closed shell ground state is always singlet) S=0, 2S+1 = 1. For a doublet, S=1/2, i.e., (1 unpaired electron), 2S + 1 = 2; and for triplet 2S+1 = 3 (2 unpaired electrons with z component electron spin quantum numbers, m_s = -1, 0, 1).

Next is a list of ***atom symbols or atomic numbers and coordinates*** given as either a set of x,y,z values or by a ***Z-matrix.*** Important: numerical coordinates **must have decimal points,** with spaces between. Exact positioning does not matter.

The list of atoms and coordinates **must end with a blank line**

“Optimizing” geometry, keyword = opt

This means the program will do a series of variation calculations, compute the force on each atom and move the atoms accordingly a little bit, and repeat the process until ***forces are essentially zero*** on each atom.

Will this process find the lowest energy geometry for a molecule???

Outline -3

8. Display MOs

9. Vibrations

Examples

create GFP

benzene normal modes

PBC