Introduction to GaussViewW

GaussView is the affordable, full-featured graphical user interface for *Gaussian 03* in the Windows environment.

GaussViewW Features

GaussView 3.0 makes using Gaussian 03 simple and straightforward.
With *GaussViewW* you can construct molecular systems of interest quickly and efficiently using its molecule building facility. You can also use it to set up and run *Gaussian* calculations. *GaussViewW* can visualize a variety of different Gaussian results, including:

- Optimized structures.
- Molecular orbitals.
- Electron densities, electrostatic potentials and other surfaces.
- IR and Raman spectra and the associated normal modes.
- Animated geometry optimization, IRC and trajectory results

How to use each of these visualizations is explained in each of the relevant lab files.

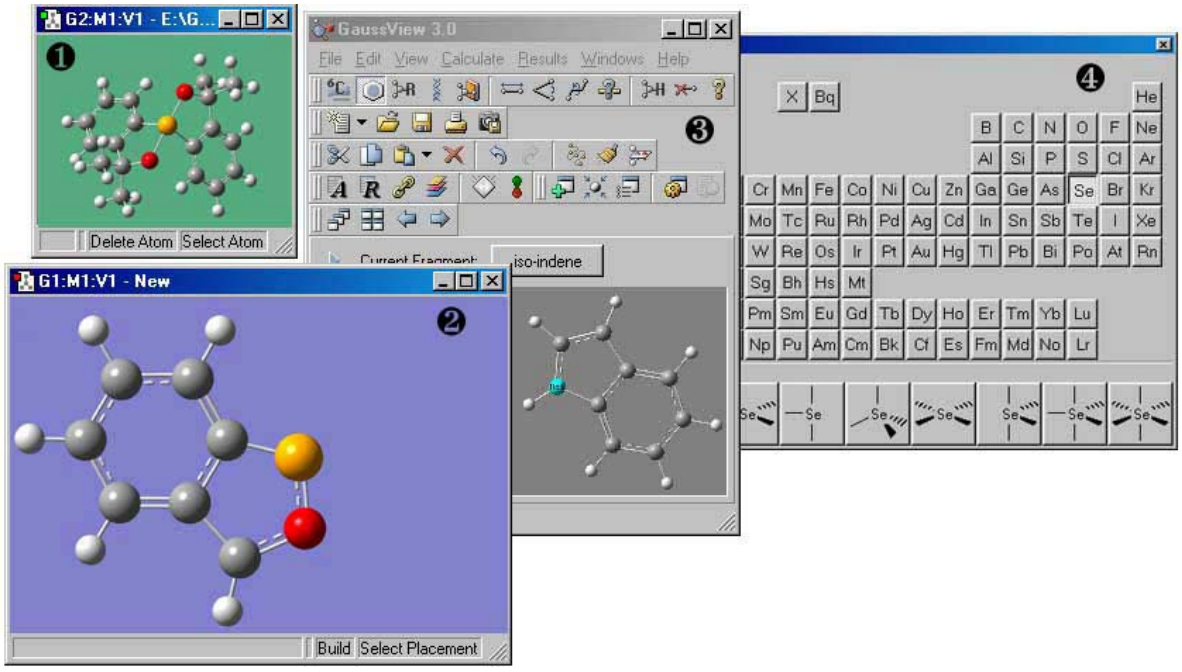

Fig A. (1) not relevant (2) where you build the molecule (3) the main GaussView window (4) the elements and fragments to be use in building the molecule

Building a molecule using GaussViewW

The GaussViewW visualization program of Gaussian can be used to construct starting point geometry for molecular calculations. The GaussViewW program can be used only in Windows environment. After opening GaussViewW you will find two windows, the main window, Fig A(3), and a small blue window, Fig A(2). In this program there are several options represented by icons placed on the Toolbar in the usual window format, Fig A(3). Each option (icon) purpose can be found under the "help" menu.

- Go to "GaussViewW help", Fig A(3), and press the left mouse button (L-click), a GaussViewW help window will be opened. On the left part of this window you will find the contents of the help.

- Go to the "Finding the Help You Need" and L-click the plus sign (+) next to it.

- Go to "Index of Icons and Menu Path" and L-click. A table of the icons and their purpose in life will open on the right part of the window.

In the main window, Fig A(3), you will see each time the different fragment (e.g. atom, molecular fragment) of the molecule which you are about to add. In the small blue window, Fig A(2), you will construct and see the molecule. To build a molecule it is best to open also a "builder" window, although all its functions can also be accessed from the Toolbar of the main window.

- Go to "view" menu and L-click the "builder" option, a "builder" window will open.

- To start drawing press the "Element Fragment" icon (the ^{6}C icon). This opens a window displaying the periodic table of the elements, Fig A(4). In order to keep this window open after choosing an atom you must change the orientation of the "pin", on the upper left side of the periodic table, so that the "window stays up".
- Choose the desired atom using the L-click. Make sure that the atom or fragment you want to add is the one that is marked on the lower part of

the periodic table, (there are single atoms and also more complicated molecular fragments). You can view the fragment you choose, before adding it, in the main GaussViewW window (Fig A(3)).

- Next, place the fragment, using the L-click, in the small blue window.

- After adding all desired atoms (excluding hydrogens) you can start bonding them as you wish using the "Modify Bond" option in the "Builder". You do this by pressing the "Modify Bond" icon then choosing two atoms by L-clicking on them in the small blue window. The two chosen atoms change color and are marked as [1] and [2]. In addition, a new window "Semichem SmartSlide" will open. In this window you select the bond order. You can also change the bond length but this is not needed for standard molecules in equilibrium (as we shell see below). Note that it is essential to press the "OK" push button after choosing the bond.

- After connecting all the main atoms in the desired way, you can add hydrogen atoms by using the "Add Valence" option on the "Builder" window. Press the "Add Valence" using the L-click then press on one of the atoms in the small blue window. Each L-click used in this way adds one hydrogen atom.

- You can remove atoms from the structure by using the "Delete Atom" icon on the "Builder" window. L-click this icon, then L-click the atom that you wish to remove.

- After all atoms are placed in the small blue (structure) window, L-click the "Clean" button in the "Builder" window in order to adjust molecular geometry according to a predefined set of rules. This adjusts the structure to a form closer to its actual geometry, as we expect from knowledge or intuition. Now the molecular structure is done and can

be used as a suitable starting geometry for a molecular optimization calculation.

- The Cartesian and Z-matrix representations of the molecular geometry can be viewed using the “Atom list editor” icon on the main GaussViewW Toolbar.

- Save the data file that you created in this way in your directory. It may be used as an input file for Gaussian calculation.

- You may also send a Gaussian job from the GaussView, see details below.

Running Gaussian "Job" using GaussViewW

We may use the GaussView program to prepare and send a Gaussian "jobs". The job parameter can be defined and adjusted on the GaussView screen. In this way we can make any desired Gaussian calculation from the GaussView interface.

How to start a Gaussian calculation after you built the desired molecule or molecules:

- L-click on the "calculation" option in the GaussView main window menu.

- L-click on the "Gaussian" option; a new window will than pop-up, the "Gaussian Calculation Setup" window, Fig B.

- This window has several options spread in two toolbars and fields.

- Before submitting a job one needs to adjust parameters, to indicate the type of calculation one desire. All Gaussian input parameters will appear above the upper toolbar; it includes "Title", "Keywords" and "Carge/Mult" categories, see Fig B. This input presentation appears in the same format as the usual Gaussian input file (one made without GaussView). The chosen parameters will be shown

spontaneously according to the choices you will make; how to make these choices is explained below. You need to check these parameters before submitting a job.

Adjusting parameters using the upper toolbar:

- Select "Job Type" option. Here you may chose the type of calculation you want to perform, e.g. energy calculation, structure optimization, NMR, etc.

- Next go to the "Method" option, Fig B(1). Here you choose the level of calculation, e.g., Hartree-Fock, DFT, etc. You may choose a restricted or unrestricted calculation, and, if you chose the DFT option a new options 'inside field' will pop-up for choosing the DFT functional, e.g. B3LYP. Here you also choose the basis set you whish to use. Eventually, you need to indicate the charge and multiplicity of the chemical system under investigation.

- The next option is the "Title": it is not necessary to write a title, but it is highly recommended. Latter, when looking at the results, the title may help you remember what was going on and if there is something important.

- The "Link 0" option is not relevant to us.

- Next is the "General" option, where here you may specify certain information, e.g. if you want additional (than the usual) printing, or should Gaussian ignore symmetry or use it. Usually it is helpful to use symmetry to reduce the calculation time; however it can be some times problematic. For example, when calculating transition state of molecular reactions may use certain symmetry as a starting input, but during the minimization search process the molecule changes geometry and no longer has that certain symmetry. In such cases it is better to disregard symmetry altogether.

- ❖ The Guess, NBO and PBC options in the upper toolbar are not relevant to us at this point.

- ❖ The last options in the upper toolbar is 'Solvation', Fig B(2). If calculation in a solvent, instead of vacuum, is desired you can do it here. You may choose the different salvation approximation method, the solvent or alternatively the associated dielectric constant.

- Below the upper toolbar there is a spatial place (field) for "Additional Keyword", Fig B(3), here you may specify any information not available in the toolbar options. For example, SCF convergence criteria; in our calculation we whish to achieve high accuracy with good (tight) convergence of the iterative procedure, to do this it is necessary to add the "Additional Keyword": SCF=Tight. Another popular "Additional Keyword" that you may use is: POP=Full (full printing of the population analysis in the output file).

- Below the "Additional Keyword" option there is another toolbar, Fig B(3). In the lower toolbar there are two important keys the "Submit" and "Edit" buttons.

- Using the "Edit" option saves your input data and opens a "WordPad" window (an editor). All parameters can be addressed and modified as you wish using the editor instead of the graphic interface. There are few calculation options that cannot be turned on in the usual GaussView way, or you may not know how to turn them on; you can do it using the editor, write them manually.

- Submitting jobs: After we specified all we need from Gaussian and our "input" is ready we need to send the Job using the "Submit" option in the lower toolbar. L-click on the "Submit" will open Gaussian after saving the input file.

- A Gaussian window is now open and it should be "working" until it is finished, it is now possible to see the Gaussian or close it and only see the output in GaussView.

- The output file: the name of the output file is chosen automatically to be the same as the input file but with CAPITAL letters and, of course, with a different ending. The input files made with GaussView will have the xxx.gjf ending. The output file will have the XXX.LOG ending.

- It is now possible to open the output file and analyze the results you have obtained. Good luck.

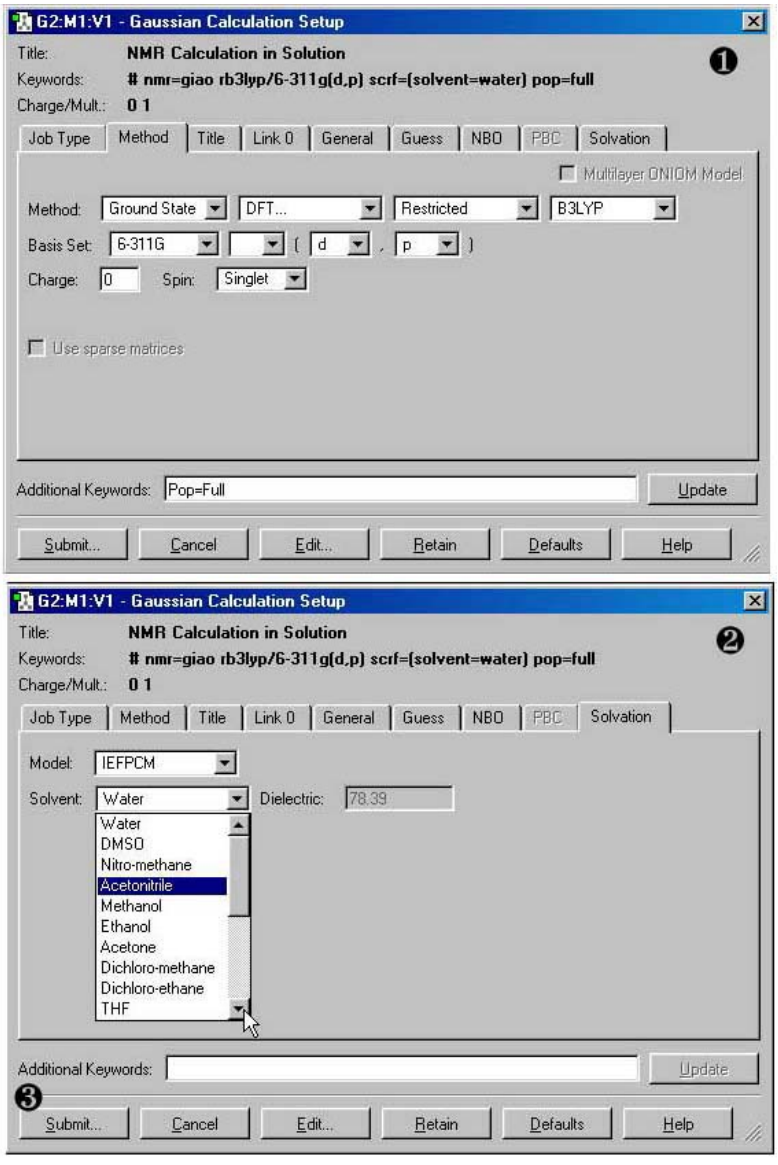

Fig B. Gaussian Calculation Setup window (1) the method option (2) the solvation option (3) additional keywords field, and the lower Toolbar

Example: setting a Gaussian Job using GaussViewW

In Fig. B we can see an example for setting Gaussian calculation. We can see all the job information from the above 'Title , Keywords, Charge/Mult' specification.

- The Title is: "NMR in solution" it was written in the 'Title' option in the upper Toolbar. Indeed, we can see it from the Keywords specification.
- From the Keywords we can see first that we request the 'normal' printing level (#), it is the default. If additional printing information is required on the output, it can be done from the 'General' option in the upper Toolbar. If terse (reduced) output is requested one need to use the 'Edit' option in the lower Toolbar and write in the Keyword: #T, instead of just #.
- Next, we request to do NMR calculation using the gauge-including atomic orbitals (GIAO, for details on the method see lab 5); it was selected from the 'Job Type' option. There are many types of jobs specified in the 'Job Type' option; there are also several NMR calculation methods.
- Next are the 'Method' option keywords, these keywords are shown in Fig B(1). We request a DFT calculation, restricted (suitable for singlet states), with the B3LYP exchange correlation functional; thus we have the 'rb3lyp' keyword.
- We continue in choosing the basis set, it is 6-311G(d,p).
- Last from the 'Method' option, we choose to calculate a neutral molecule (charge=0) with a singlet multiplicity. These appear below the 'Keywords' as 'Charge/Mult: 0 1'.
- Next is the solvation, Fig B(2), SCRF is the keyword which requests that the calculation be performed in the presence of a solvent, it appear when we choose a solvation model. Here we choose the Polarizable Continuum model (PCM) using integral equation formalism (IEFPCM) (see solvation lab).
- The solvent is also chosen here, it is water so we have scrf=(solvent=water) in the Keyword. Although as we can see from Fig B(2) the solvent may soon be changed to Achetonitrile, and so we will have scrf=(solvent= Achetonitrile) ☺
- Finally, we have from the "Additional Keyword" pop=full (full printing of the population analysis in the output file) as can be seen in Fig B(1).