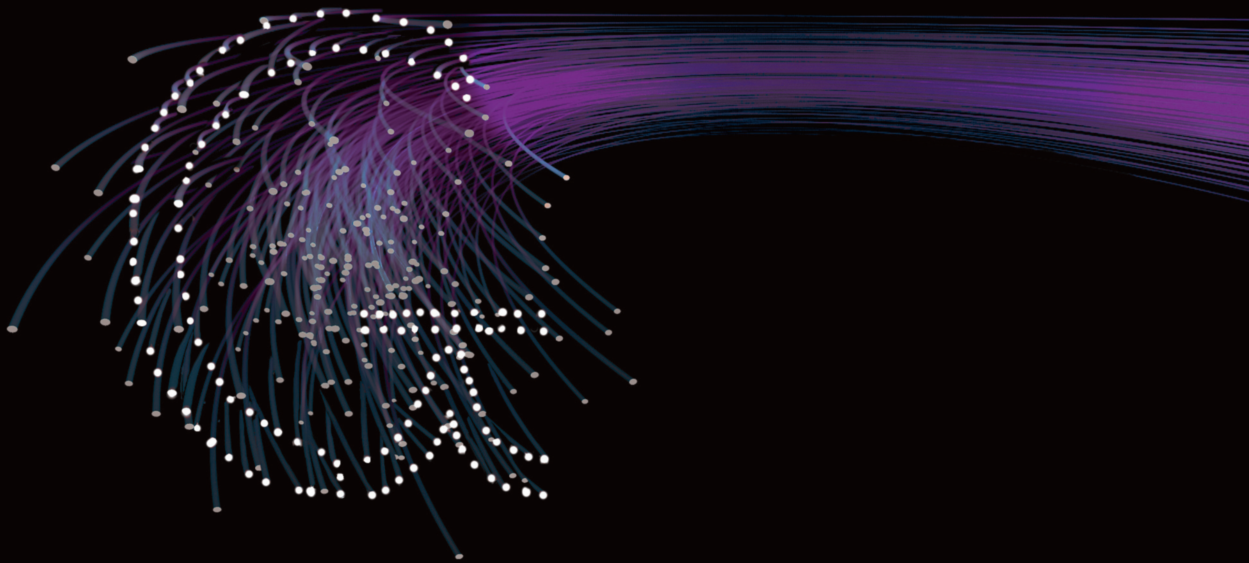
# GaussView 5 Reference



# GaussView 5
# Reference

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# Table of Contents

List of Figures . . . . . vii

Introduction . . . . . 1
    Typographic Conventions . . . . . 1

GaussView Basics . . . . . 2
Molecules, Molecule Groups and Views . . . . . 3
    Customizing MultiView Windows . . . . . 5
    Animating Multiple Structures . . . . . 6
Using the Mouse . . . . . 6
    Limiting Mouse Actions to One Fragment . . . . . 6
GaussView Menus . . . . . 7
Table of Icons and Menu Items . . . . . 7
GaussView Preferences . . . . . 12
    Specifying GaussView Window Behavior . . . . . 13
    Modifying Icon Sizes . . . . . 13
Displaying GaussView Tips . . . . . 14

Building Molecules . . . . . 15
Placing Elements and Fragments . . . . . 15
    The Element Fragments Palette . . . . . 15
    The R-Group Fragments Palette . . . . . 16
    The Rings Palette . . . . . 16
    The Biological Fragments Palette . . . . . 17
        Making Palettes Sticky . . . . . 17
    Placing a Fragment in a Centroid Position . . . . . 17
    Undo and Redo . . . . . 18
Viewing and Adjusting Structure Parameters . . . . . 18
    Inquire Mode . . . . . 18
    Semichem SmartSlides . . . . . 19
        The Bond SmartSlide . . . . . 19
        The Angle and Dihedral SmartSlides . . . . . 20
    Adding and Deleting Valences . . . . . 21
    Invert About Atom (Mirror Invert) . . . . . 22
    Cleaning Structures . . . . . 22
        Clean Performance Tips . . . . . 24
    Rebonding Structures . . . . . 24
    Imposing Symmetry . . . . . 24
All About Selections: From Atoms to Fragments, Residues, Chains and Beyond . . . . . 26
    Selection-Related Toolbar Icons . . . . . 26
        Selection Keystrokes in View Windows . . . . . 26
    Selecting with the Atom List Editor and Similar Tools . . . . . 26
    Using the Atom Group Editor . . . . . 27
    The Atom Selection Editor . . . . . 28
Advanced Building Features . . . . . 29
    Using a Custom Fragment Library . . . . . 29
    The Atom List Editor . . . . . 30
        Using Sublist Filters . . . . . 33
        Defining Isotope Masses and Isotopologues . . . . . 34
    The PDB Residue Editor and The PDB Secondary Structure Editor . . . . . 34

- The Connection Editor . . . . . 35
- The Redundant Coordinate Editor . . . . . 36
- Specifying ONIOM Layers . . . . . 37
  - Confirming Layer Assignments . . . . . 39
  - Layer Display Formats . . . . . 39
- The Molecular Orbital (MO) Editor . . . . . 39
  - Modifying Orbital Occupancies, Molecular Charge and Spin Multiplicity . . . . . 41
  - Controlling the Orbitals Display . . . . . 41
  - Generating and Retrieving MOs . . . . . 42
  - Rearranging Orbital Ordering . . . . . 42
  - Miscellaneous Options . . . . . 42
- Building Periodic Systems with the Crystal Editor . . . . . 42
  - The Symmetry Panel . . . . . 43
  - The Contents Panel . . . . . 44
  - The Cell Panel . . . . . 45
  - The Reduce Panel . . . . . 47
  - The View Panel . . . . . 47
- Specifying Fragment Placement Behavior . . . . . 48

Opening, Displaying and Saving Molecules and Views . . . . . 51

Customizing and Manipulating Molecule Views . . . . . 51
- Centering the Molecule . . . . . 51
- Viewing Optional Display Items . . . . . 51
- Molecule Positioning Tools . . . . . 52
- Molecule Display Formats . . . . . 52
  - The General Panel . . . . . 52
- The Molecule Panel . . . . . 53
  - The Text Panel . . . . . 55
- Customizing Display Colors . . . . . 56
  - Specifying Colors . . . . . 56
- Adding and Synchronizing Views . . . . . 57
- Selecting View Windows . . . . . 57

Working with Molecules and Files . . . . . 58
- Pasting Molecules into the View Window . . . . . 58
- File Drag and Drop under Windows . . . . . 58
- Adding a Model . . . . . 58
- Opening Existing Models and Other Files . . . . . 59
- Additional File Open Options . . . . . 60
- Accessing Recent and Related Files . . . . . 60
- Viewing the Input File for the Current Results . . . . . 61
- Saving Molecules . . . . . 61

Printing and Saving Images . . . . . 61
- Printing . . . . . 61
- Capturing Images and Saving Image Files . . . . . 62
- Saving Movies . . . . . 63
- Saving Plot and Spectrum Images . . . . . 64

Specifying Default File Locations . . . . . 64
- Specifying File Associations Under Windows . . . . . 65

Setting up and Running Gaussian Jobs . . . . . 66

The Gaussian Calculation Setup Window . . . . . 66
- The Job Type Panel . . . . . 67
- The Method Panel . . . . . 67
- The Title Panel . . . . . 68
- The Link 0 Panel . . . . . 68

- The General Panel. . . . . . . . . . 69
- The Guess Panel . . . . . . . . . . 70
- The NBO Panel . . . . . . . . . . 71
- The Solvation Panel . . . . . . . . . . 71
- The PBC Panel. . . . . . . . . . 71
- The Additional Input Panel. . . . . . . . . . 72

Special Considerations for Various Gaussian Job Types . . . . . . . . . . 72
- Transition Structure Optimizations: Opt=QST2 and Opt=QST3 . . . . . . . . . . 72
  - Verifying and Specifying Atom Equivalences . . . . . . . . . . 72
- Calculations on Polymers, Surfaces and Crystals . . . . . . . . . . 72
- Multi-Layer ONIOM Calculations. . . . . . . . . . 72
  - Assigning Atoms to Layers . . . . . . . . . . 72
  - Assigning Molecular Mechanics Atoms Types . . . . . . . . . . 72
  - Defining Link Atoms . . . . . . . . . . 72
  - Specifying the Model Chemistry for Each Layer. . . . . . . . . . 73
- Specifying CASSCF Active Spaces Using Guess=Permute . . . . . . . . . . 73
- Modifying Redundant Internal Coordinates (Geom=ModRedundant) . . . . . . . . . . 73
- Freezing Atoms During Geometry Optimizations . . . . . . . . . . 73
- Selecting Normal Modes for Frequency Calculations (Freq=SelectNormalModes) . . . . . . . . . . 74
- Calculating NMR Spin-Spin Coupling (NMR=(SpinSpin,ReadAtoms)). . . . . . . . . . 74
- Specifying Fragment-Specific Charges and Spin Multiplicities . . . . . . . . . . 74

Setting Defaults for Gaussian Jobs . . . . . . . . . . 75
- Defining Calculation Schemes . . . . . . . . . . 75

The Quick Launch Feature . . . . . . . . . . 75

Viewing and Controlling Gaussian Jobs . . . . . . . . . . 76

Specifying How the Gaussian Program is Executed . . . . . . . . . . 76

Viewing Gaussian Results . . . . . . . . . . 79

Calculation Summary. . . . . . . . . . 79

Displaying Atomic Charges Computed in Gaussian. . . . . . . . . . 79
- Charge Distribution Preferences . . . . . . . . . . 80

Displaying Surfaces and Contours . . . . . . . . . . 81
- Generating and Manipulating Cubes . . . . . . . . . . 82
- Displaying Surfaces . . . . . . . . . . 83
- Mapped Surfaces. . . . . . . . . . 83
- Customizing Surface Displays . . . . . . . . . . 84
- Displaying Contours . . . . . . . . . . 85
  - Defining the Contour Plane . . . . . . . . . . 86

Displaying Vibrational Modes and IR/Raman Spectra. . . . . . . . . . 87
- Displaying the Spectrum . . . . . . . . . . 88
- Vector-Based Displays . . . . . . . . . . 88
  - Using Manual Displacement Display Mode . . . . . . . . . . 89
- Comparing Spectra for Isotopologues. . . . . . . . . . 89
- Frequency-Dependent Calculation Results . . . . . . . . . . 90

Displaying NMR Spectra . . . . . . . . . . 91

Displaying UV-Visible Spectra. . . . . . . . . . 91

Viewing Optimization Results and Other Structure Sequences . . . . . . . . . . 92
- Viewing 3D Plots of 2-Variable Scan Calculations . . . . . . . . . . 93
- Plotting Additional Properties . . . . . . . . . . 93
- Correcting Plot Discontinuities . . . . . . . . . . 93

Manipulating and Customizing Plots and Spectra . . . . . . . . . . 94
- Customizing Plots and Spectra. . . . . . . . . . 95

Saving Plot Data . . . . . . . . . . 96

Index . . . . . . . . . . 99

# List of Figures

Figure 1. GaussView on the Desktop . . . . . 2
Figure 2. Toolbar Context Menu . . . . . 3
Figure 3. GaussView Toolbars in Standalone Mode . . . . . 3
Figure 4. A Molecule Group Containing 12 Molecules . . . . . 4
Figure 5. Color Icons from 2 Different Views . . . . . 5
Figure 6. View Window Context Menu . . . . . 5
Figure 7. Restoring Default Preferences . . . . . 13
Figure 8. Window Behavior Preferences . . . . . 13
Figure 9. Customizing Icon Sizes . . . . . 14
Figure 10. GaussView Tips . . . . . 14
Figure 11. The Element Fragments Palette . . . . . 15
Figure 12. The R-Group Fragments Palette . . . . . 16
Figure 13. The Ring Fragments Palette . . . . . 16
Figure 14. Selecting Biological Fragments. . . . . . 17
Figure 15. Placing a Centroid Atom in $C_{60}$ . . . . . 17
Figure 16. Inquire Mode Display . . . . . 18
Figure 17. The Bond SmartSlide . . . . . 19
Figure 18. Bond Length Modification Options . . . . . 20
Figure 19. Angle and Dihedral SmartSlides . . . . . 20
Figure 20. Bond Angle Modification Options . . . . . 21
Figure 21. Deleting a Dangling Bond (Open Valence) . . . . . 22
Figure 22. Inverting a Structure About an Atom. . . . . . 22
Figure 23. Customizing the Clean Function. . . . . . 23
Figure 24. Imposing Symmetry on a Molecular Structure . . . . . 25
Figure 25. Symmetry-Related Status Bar Displays. . . . . . 25
Figure 26. The Atom Group Editor . . . . . 27
Figure 27. The Atom Selection Editor . . . . . 28
Figure 28. The Custom Fragments Window. . . . . . 29
Figure 29. The Atom List Editor . . . . . 30
Figure 30. Additional Atom List Editor Columns . . . . . 31
Figure 31. Assigning MM Charges with the Atom List Editor . . . . . 32
Figure 32. Creating Sublist Filters . . . . . 33
Figure 33. The PDB Residue and PDB Secondary Structure Editors . . . . . 35
Figure 34. The Connection Editor . . . . . 36
Figure 35. The Redundant Coordinate Editor . . . . . 37
Figure 36. Assigning Atoms to ONIOM Layers. . . . . . 38
Figure 37. Selecting Atoms for Layer Assignment by PDB Residue . . . . . 38
Figure 38. The MO Editor . . . . . 39
Figure 39. The MO Editor’s New, Calculation and Diagram Panels . . . . . 40
Figure 40. Degenerate Orbitals in the MO Editor . . . . . 41
Figure 41. The PBC Symmetry Panel. . . . . . 43
Figure 42. The PBC Contents Panel. . . . . . 44
Figure 43. The PBC Cell Panel . . . . . 45
Figure 44. Modified and Rebonded GaAS Unit Cell . . . . . 46
Figure 45. The PBC Reduce Panel . . . . . 47
Figure 46. The PBC View Panel . . . . . 48
Figure 47. Fragment Placement Restrictions . . . . . 49
Figure 48. Structure Options After a Fragment Placement . . . . . 49
Figure 49. Displaying Cartesian Axes . . . . . 51

Figure 50. The Positioning Toolbar . . . . . 52
Figure 51. Display Format General Panel . . . . . 53
Figure 52. The Fog Depth Display Feature . . . . . 53
Figure 53. The Display Format Molecule Panel . . . . . 54
Figure 54. A CPK-Like Display. . . . . . 54
Figure 55. Tube Display Formats . . . . . 55
Figure 56. The Text Panel of the Display Format Dialog . . . . . 55
Figure 57. Customizing GaussView Colors . . . . . 56
Figure 58. Surface Coloring Preferences . . . . . 57
Figure 59. GaussView Fields in the Open File Dialog. . . . . . 59
Figure 60. File Opening Options . . . . . 60
Figure 61. GaussView Fields in the Save File Dialog . . . . . 61
Figure 62. GaussView Print Preferences . . . . . 62
Figure 63. GaussView Fields in the Save Image Dialog . . . . . 62
Figure 64. Image Capture Preferences. . . . . . 63
Figure 65. Specifying Default Directory Locations . . . . . 64
Figure 66. Specifying Windows File Associations . . . . . 65
Figure 67. The Gaussian Calculation Setup Dialog . . . . . 66
Figure 68. Adding an Option via the Additional Keywords Field . . . . . 67
Figure 69. The Method Panel . . . . . 68
Figure 70. Entering a Custom Basis Set Keyword . . . . . 68
Figure 71. The Link 0 Panel. . . . . . 69
Figure 72. Selecting General Gaussian Options . . . . . 69
Figure 73. Gaussian Initial Guess Options . . . . . 70
Figure 74. The NBO Panel. . . . . . 71
Figure 75. The Solvation Panel . . . . . 71
Figure 76. The PBC Panel . . . . . 71
Figure 77. Setting Up a Gaussian Input File for an ONIOM Job . . . . . 73
Figure 78. Specifying Per-Fragment Charge and Spin . . . . . 74
Figure 79. Viewing and Modifying Calculation Schemes. . . . . . 75
Figure 80. The Job Manager Dialog . . . . . 76
Figure 81. Job Setup Preferences . . . . . 77
Figure 82. Running Gaussian via a Script . . . . . 77
Figure 83. Summary of a Gaussian Calculation . . . . . 79
Figure 84. Displaying Atomic Charges . . . . . 80
Figure 85. Charge Distribution Preferences . . . . . 81
Figure 86. The Surfaces and Contours Dialog . . . . . 81
Figure 87. The Generate Cubes Dialog . . . . . 82
Figure 88. Creating a Cube as the Difference of Two Densities . . . . . 82
Figure 89. Example GaussView Surfaces. . . . . . 83
Figure 90. Creating a Mapped Surface. . . . . . 84
Figure 91. Customizing a Surface Display . . . . . 85
Figure 92. Example Contour Plot. . . . . . 85
Figure 93. The Generate Contours Dialog . . . . . 86
Figure 94. Specifying the Desired Contour Plane . . . . . 86
Figure 95. Running FreqChk to Perform Vibrational Analysis. . . . . . 87
Figure 96. The Display Vibrations Window . . . . . 87
Figure 97. GaussView Spectra Displays. . . . . . 88
Figure 98. Displaying the Displacement Vector and Dipole Derivative Unit Vector . . . . . 89
Figure 99. Setting Up Isotopologues and Comparing Normal Modes. . . . . . 90
Figure 100. Specifying a Specific Frequency . . . . . 90
Figure 101. NMR Spectrum Display . . . . . 91
Figure 102. Displaying NMR Chemical Shifts . . . . . 91
Figure 103. Example UV-Visible Spectrum Display . . . . . 91

Figure 104. Retrieving Intermediate Results from Optimizations and Similar Jobs . . . . . . . . . . . . . . . . . . . . . . . . . . . . 92
Figure 105. Plots from a Geometry Optimization . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 92
Figure 106. Results Plot for a PES Scan over 2 Variables . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 93
Figure 107. Creating An Additional Plot . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 93
Figure 108. The Plots Menu. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 94
Figure 109. Zooming In on a Spectrum . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 94
Figure 110. The Plot/Spectrum Context Menu and Save Data Range Fields . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 95
Figure 111. Customizing a Plot/Spectrum . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 95

# Introduction

GaussView is a graphical user interface designed to help you prepare input for submission to Gaussian and to examine graphically the output that Gaussian produces. GaussView is not integrated with the computational module of Gaussian, but rather is a front-end/back-end processor to aid in the use of Gaussian. GaussView provides three main benefits to Gaussian users.

First, through its advanced visualization facility, GaussView allows you to rapidly sketch in even very large molecules, then rotate, translate and zoom in on these molecules through simple mouse operations. It can also import standard molecule file formats such as PDB files.

Secondly, GaussView makes it easy to set up many types of Gaussian calculations. It makes preparing complex input easy for both routine job types and advanced methods like ONIOM, STQN transition structure optimizations (i.e., **Opt=QST2/QST3**), CASSCF calculations, periodic boundary conditions (PBC) calculations, and many more. You can also use GaussView to launch jobs as well if Gaussian is installed on the same computer. Lastly, you can define default and named calculation templates—known as schemes—to speed up the job setup process.

Finally, 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.

This book provides a reference to all of GaussView's features. Each of the program's features is documented in detail. Items are arranged into several groups based on their general purpose. Within a group, items are arranged in a logical progression, beginning with the simplest, most widely used ones and then progressing to more complex and unusual capabilities.

Several hands-on tutorials on various GaussView features are included in the online help. Select the Tutorials topic from the main help screen in order to access them.

### Typographic Conventions

In order to locate the specific information in which you are interested, consult the index for the desired topic or particular dialog. Within this text, palettes and dialogs are referred to by their title text; the names of items within them are set in **Blue** type. **Menu items** are indicated by the form **Menu=>Item**. **Buttons** are referred to and indexed as the **Name** button. **Dialog names** are set off in **Black**. Gaussian keywords and options, like **Opt=QST2**, are set in **Purple** (but names CASSCF and ONIOM are set in normal type when they are discussed as general methods). See the table beginning on page 7 for a list of button names, menu path-button equivalences and keyboard shortcuts.

# GaussView Basics

The main GaussView interface consists of several windows, in addition to other dialogs which appear in the course of working. Figure 1 illustrates a simple session in which the user has just started to build a molecule.

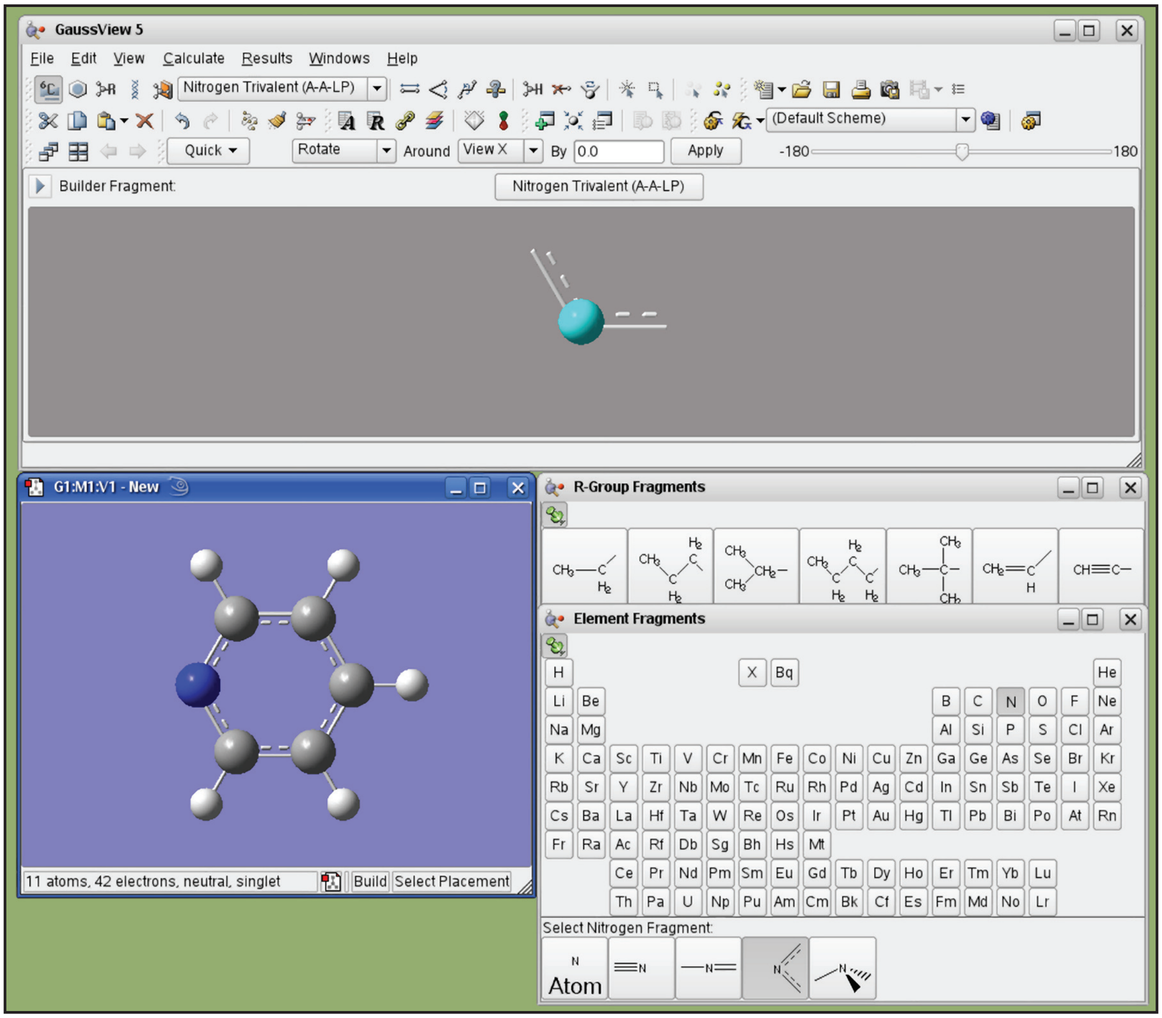

GaussView 5
File Edit View Calculate Results Windows Help
Nitrogen Trivalent (A-A-LP)
(Default Scheme)
Quick
Rotate
Around
View X
By
0.0
Apply
-180
180
Builder Fragment:
Nitrogen Trivalent (A-A-LP)
G1:M1:V1 - New
11 atoms, 42 electrons, neutral, singlet
Build
Select Placement
R-Group Fragments
Element Fragments
Select Nitrogen Fragment:
Atom

**Figure 1. GaussView on the Desktop**

*Several GaussView features are visible here. At the top, we see the main GaussView control panel, containing the menu bar, a variety of toolbars, and the Current Fragment window. Below this, on the right, are the palettes used to select functional groups and individual atoms for addition to a molecule (note that these can function in a modal or amodal mode, according to user preference). At the bottom left is the active View window containing the molecule being built.*

The GaussView interface consists of these main components:

- The control panel containing the menu bar and **Current Fragment** display.
- Various toolbars. By default, these are placed below the menu bar in the control panel, but they may also be detached if desired (see Figure 3). They may also be rearranged within the control panel as desired (so your window may differ from the illustration in Figure 1).
- One or more molecule View windows.
- Dialogs corresponding to the various GaussView features.
- Preferences which control various aspects of the program's functioning.

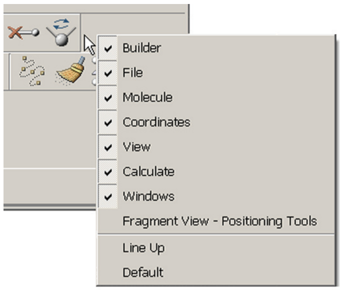


Figure 2. Toolbar Context Menu

The toolbars that appear by default under the menu bar in the GaussView control panel are illustrated individually in Figure 2. The **Builder** toolbar can also appear as a standalone palette, as it does in Figure 2. You can open it with **View=>Builder**. You can detach an individual toolbar from the main toolbar by grabbing the handle and dragging it out of the toolbar area. To reattach a standalone toolbar, either drag it back into the main toolbar or double click it.

If you right click in the grey area within any toolbar, you will bring up the Toolbar context menu. The first section of the list contains the names of the toolbars that are available in that window. Selecting one of the toolbar names from the list will toggle it between its visible and hidden states. The **Line Up** option causes the toolbars to move to eliminate empty space between them, and the **Default** option restores the default configuration for that toolbar (when applicable).

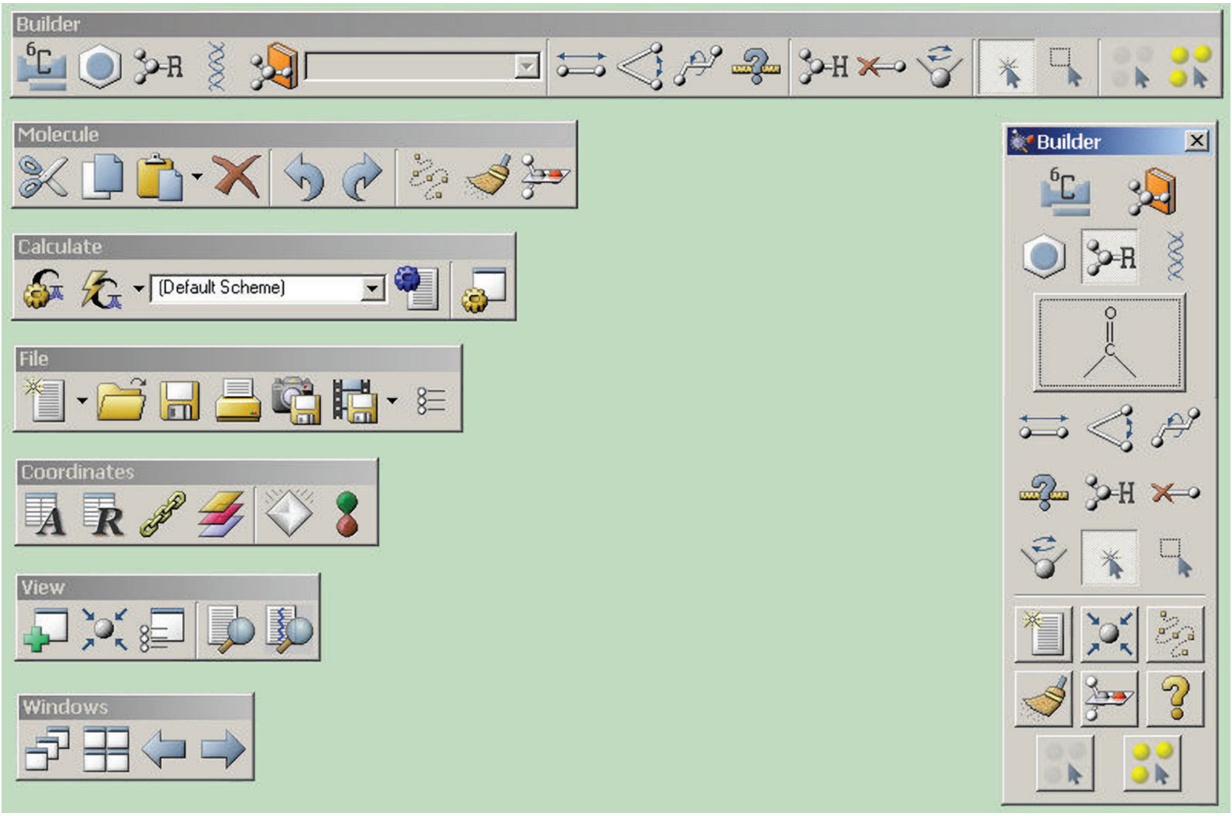


Figure 3. GaussView Toolbars in Standalone Mode

*The Builder palette on the right is revealed with the View=>Builder menu path.*

## Molecules, Molecule Groups and Views

GaussView uses these constructs to organize the many molecules which are being utilized at any given time:

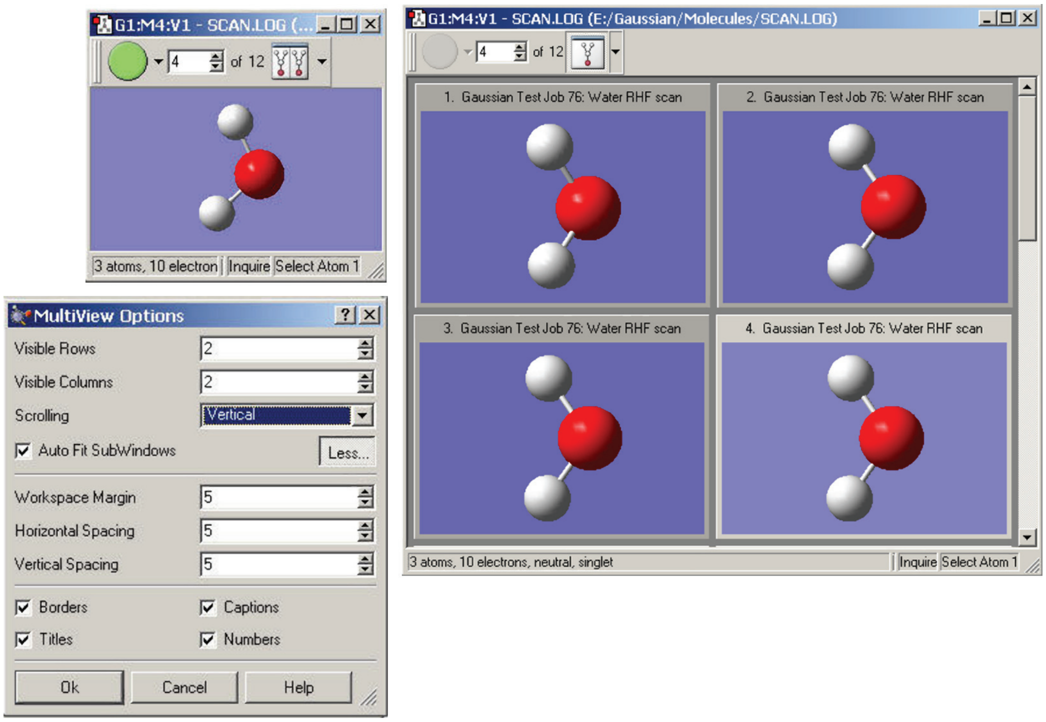
- A *molecule* is most often a single molecule being worked on in isolation from other ones that may also be open. A molecule generally corresponds to a single file stored on disk. These are also sometimes referred to as *models*. Note that a molecule in this sense may contain more than one chemical species (i.e., “molecules” in the usual chemical sense).
- If there is more than one window open for the same molecule, the various different ones are referred to as *views*. Accordingly, a View window displays a molecule, and different views—and View windows—can display different orientations and properties of the same molecule.

- A *molecule group* is a collection of one or more molecules that are worked on as a unit. Molecule groups containing more than one molecule display each one in a separate subwindow of a combination View window (see Figure 4). Molecule groups are also referred to as *model groups*.

For molecule groups containing more than one molecule, there are two display modes. *Single-view mode* displays a single molecule at a time. The current molecule number appears in the toolbar. Clicking the single/multiview icon brings up *multiview mode* in which several molecules can be viewed at one time. Individual molecule views are contained within the larger multiview window. The molecule number is shown in the title bar of each frame. The currently active molecule is shown with a slightly lighter background to distinguish it from the other molecules and is the one involved in atom selections or in the dialogs. Clicking on one of the individual molecule windows that is not the active molecule window will cause it to become the active molecule. In the event that not all of the individual molecules can fit in the View window, a scroll bar at the bottom of the View window allows one to move between the different molecules.

Clicking on the small triangle to the right of the single view/multiview icon reveals a small menu containing these items:

- **Options**: Opens the **MultiView Options** dialog (illustrated in the bottom left of Figure 4 and discussed below).
- **Fit**: Resize all individual molecule frames so all are visible in the window.
- **Synchronize**: Link all frames so that mouse actions in one affect all of them (e.g., rotations). By default, each view is independent.


G1:M4:V1 - SCAN.LOG (...
4
of 12
3 atoms, 10 electron
Inquire
Select Atom 1
G1:M4:V1 - SCAN.LOG (E:/Gaussian/Molecules/SCAN.LOG)
4
of 12
1. Gaussian Test Job 76: Water RHF scan
2. Gaussian Test Job 76: Water RHF scan
3. Gaussian Test Job 76: Water RHF scan
4. Gaussian Test Job 76: Water RHF scan
3 atoms, 10 electrons, neutral, singlet
Inquire
Select Atom 1
MultiView Options
Less...
Ok
Cancel
Help

Visible Rows: 2
Visible Columns: 2
Scrolling: Vertical
☑ Auto Fit SubWindows
Workspace Margin: 5
Horizontal Spacing: 5
Vertical Spacing: 5
☑ Borders ☑ Captions
☑ Titles ☑ Numbers

**Figure 4.** A Molecule Group Containing 12 Molecules

*The multiview controls in the toolbar appear only when there is >1 molecule in a molecule group. The single/multiple view icon toggles between single-window (upper left) and multi-window view (right). The MultiView Options dialog controls the layout and behavior of multiview display mode.*

View window title bars display information about the current molecule group, molecule and view: each distinct molecule group is identified by an icon whose color is uniquely associated with it. Figure 5 shows the color icons from two different view windows (each corresponding to a different molecule group). All dialogs that are directly associated with that molecule group will use the same color icon to visually associate themselves with their parent molecule group (including new views created using **View=>Add View**). This color icon is also used to identify the molecule group in the **Windows** menu.

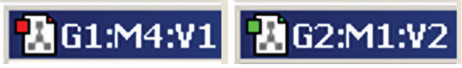

G1:M4:V1
G2:M1:V2

**Figure 5.** Color Icons from 2 Different Views

*The icon on the left corresponds to the 4th molecule in the 1st molecule group (red), while the one on the right is the 2nd view of the 1st molecule in the second molecule group (green). This same color icon will appear in all dialogs associated with that molecule. For some operating systems, the color icon is located in the status bar.*

In addition to its color icon, each View window is uniquely identified by its group/molecule/view identifier. This identifier consists of the molecule group (**G**), the molecule number (**M**), and the view number (**V**). Each of the molecules in a molecule group are numbered sequentially starting at 1. If a molecule in the group is deleted, the molecules are renumbered to maintain a continuous sequence.

Note that dialogs corresponding to molecule editing function are molecule-specific. If you activate a different View window with, say, the **Atom List Editor** open, its context does not follow. Examine the header label of a dialog in order to determine the corresponding View window.

Right clicking anywhere within a molecule window will bring up a context menu. The contents of the context menu duplicates much of the Builder, the menu bars, and the toolbars. This is provided as a convenience for the user.

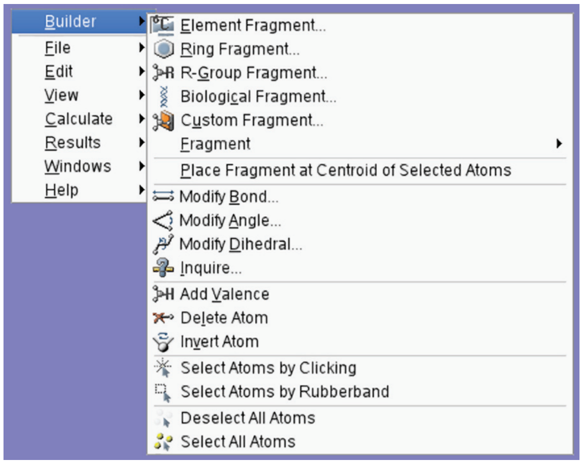

Builder
File
Edit
View
Calculate
Results
Windows
Help
Element Fragment...
Ring Fragment...
R-Group Fragment...
Biological Fragment...
Custom Fragment...
Fragment
Place Fragment at Centroid of Selected Atoms
Modify Bond...
Modify Angle...
Modify Dihedral...
Inquire...
Add Valence
Delete Atom
Invert Atom
Select Atoms by Clicking
Select Atoms by Rubberband
Deselect All Atoms
Select All Atoms

**Figure 6.** View Window Context Menu

*Each of the options on the context menu brings up a submenu containing related items.*

## Customizing MultiView Windows

The various controls in the **MultiView Options** dialog have the following uses:

- **Visible Rows** and **Visible Columns**: Number of rows and columns of individual frames initially appearing in a multiview window.
- **Scrolling**: Placement of scroll bars.
- **Auto Fit SubWindows**: When unchecked, resizing the multiview window does not affect the size of the individual frames, and so more of them are typically visible when the window is made larger. When checked, individual frames are resized whenever the main window is, so that the same number of frames are always visible (based on the row and column values specified).

The following controls are visible when the **More** button has been pressed:

- **Workspace Margin**, **Horizontal Spacing** and **Vertical Spacing**: Padding around the block of individual view subwindows and between the individual columns and rows (respectively).

- **Borders**, **Titles**, **Captions** and **Numbers**: When checked, **Borders** displays border on individual view frames. **Titles** and **Numbers** control whether the job title and structure number appear in each frame title bar. **Captions** controls all title bar text as a whole, and unchecking it suppresses all text regardless of the settings of the other items.

### Animating Multiple Structures

Clicking on the green run button in the toolbar for a multiview molecule group will cause the View window to show each molecule in the group sequentially and continue to cycle through the full list until stopped. This has the effect of visually animating the sequence of molecules like a movie. This can be particularly useful for animating a series of related geometries, such as a Reaction Path plot. After the green run button has been pressed, it turns into a red stop button, which will stop the animation.

The small triangle next to the animation button contains a small menu. Its **Loop** item causes the animation to loop continuously until stopped. The **Reverse** item cause the frames to be displayed in highest-to-lowest order rather than in ascending frame number order. Note that these options cannot be set while an animation is running.

The animation speed can be controlled by the user. For an individual View window, the animation delay can be changed in the **Display Format** dialog's **Molecule** tab. The default animation delay is set in the **Display Format Preferences**.

## Using the Mouse

Interaction with molecules is designed around the movements of a three-button mouse. The functions of the mouse buttons are described in the following table:

| Mouse Button | | | |
|---|---|---|---|
| 3-Button | 1,2-Button Equiv. | Action | Function |
| Left | Left | Click | Insert atom/fragment, pick atom for modification, etc. |
| | | Click (C key pressed) | Select or deselect by atom, |
| | | Drag (R key pressed) | Select or deselect via marquee. |
| | | Drag Left/Right | Rotate about Y axis. |
| | | Drag Up/Down | Rotate about X axis. |
| Center | Shift-Left | Drag | Translate molecule. |
| Right | Ctrl-Left | Drag Left/Right | Rotate about Z axis. |
| | | Drag Up/Down | Zoom in and out. |
| | | Click in an open area | Display context menu. |
| | | Shift-Click on atom | Highlight corresponding row in **Atom List Editor**. |

Note that these mouse actions are active in any molecule display (including ones in GaussView dialogs).

### Limiting Mouse Actions to One Fragment

If two items are not bonded to one another (not connected by visible chemical bonds on the screen), you can manipulate them individually on screen by holding down the Alt key and moving the cursor. When you use the Alt key, only the fragment closest to the cursor is affected. Thus Alt-Shift allows you to drag only one fragment.

## GaussView Menus

GaussView contains the following menus, which have the indicated general purposes:

- **File**: Creating, opening, printing and saving structures and movies, as well as setting GaussView preferences.
- **Edit**: Performing molecule building and configuration tasks.
- **View**: Managing and interacting with the display of molecules.
- **Calculate**: Setting up and submitting Gaussian calculations and viewing current GaussView-initiated jobs.
- **Results**: Examining calculation results, including surfaces, spectra, plots, and animations.
- **Windows**: Managing the various GaussView windows.
- **Help**: Viewing help files for GaussView and Gaussian, as well as GaussView tips.

## Table of Icons and Menu Items

The following table lists the available icons and menu items along with their functions. Most items will be described in more detail in future sections of this book. Note that on Mac OS X systems, the Equivalent Key modifier is the Command key, not the Control key.

| Icon | Name | Menu Path | Purpose | Keystroke |
|---|---|---|---|---|
| | New | File=>New | Create a new molecule (per submenu selection). | |
| | | File=>New=> Create Mol. Group | Create a new (one-member) molecule group as an empty View window. | Ctrl-N |
| | | File=>New=> Add to Mol. Group | Add a new molecule to the current molecule group. | Ctrl-Shift-N |
| | Open | File=>Open | Open files supported by GaussView. | Ctrl-O |
| | | File=>Recent Files | List of recently-opened files for easy reaccess. | |
| | | File=>Related Files | List of files related to the current molecule (e.g., input file, log file, checkpoint file, etc.) | |
| | | File=>Refresh | Reload current file in active View window. | |
| | Save | File=>Save | Save molecule(s) in the active molecule group to file(s). | Ctrl-S |
| | | File=>Save | Save any temporary files associated with Gaussian Quick Launch jobs. | |
| | Print | File=>Print | Print the contents of the active View window. | Ctrl-P |
| | Save Image | File=>Save Image File | Produce a graphics file of current View window. | |
| | Save Movie | File=>Save Movie | Save movie file, movie frame files, or both (selected via submenu). | |
| | Preferences | File=>Preferences | Specify defaults for aspects of GaussView's behavior. | |
| | | File=>Exit | Close all GaussView windows and exit application. | |
| | Undo | Edit=>Undo | Reverse the previous editing action and maintain a list of all previous actions for potential Redo. | Ctrl-Z |
| | Redo | Edit=>Redo | Reverse the previous Undo operation. | Ctrl-Y |
| | Cut | Edit=>Cut | Cut the current selection to clipboard. | Ctrl-X |

| Icon | Name | Menu Path | Purpose | Keystroke |
|---|---|---|---|---|
| | Copy | Edit=>Copy | Copy the current selection to clipboard. | Ctrl-C |
| | Paste | Edit=>Paste | Copy clipboard contents to the current model (per submenu selection). | |
| | | Edit=>Paste=>Add to Molecule Group | Add the molecule on the clipboard as a new model within the current model group. | Ctrl-V |
| | | Edit=>Paste=> Replace Molecule | Replace current molecule with clipboard contents. | |
| | | Edit=>Paste=> Append Molecule | Add molecule on the clipboard to the current model as a separate fragment | |
| | Delete | Edit=>Delete | Remove the current selection. | Ctrl-Shift-V<br>Del |
| | | Edit=>Image Capture | Copy the contents of the active View window to the clipboard. | Ctrl-I |
| | Atom List Editor | Edit=>Atom List | Edit the molecule's numerical coordinates and parameters in a spreadsheet-like dialog. | |
| | Redundant Coord. Editor | Edit=>Redundant Coordinates | Specify redundant internal coordinates for the Gaussian ModRedundant option. | |
| | Connection Editor | Edit=> Connection | Specify corresponding atoms in two related molecular structures (e.g., for Opt=QST2 or QST3 input). | |
| | Select Layer | Edit=>Select Layer | Assign atoms to layers graphically for ONIOM calculations. | |
| | | Edit=>Atom Groups | Open the **Atom Group Editor**, useful for defining fragments, ONIOM layers, frozen atoms and other atom groupings. | |
| | | Edit=>Atom Selection | Open the **Atom Selection Editor**, enabling you to perform advanced selection operations. | |
| | | Edit=>PDB Residues | Open the **PDB Residue Editor** which enables operations based on residues as defined in the originating PDB file. | |
| | | Edit=>PDB Secondary Structures | Open the **PDB Secondary Structure Editor** which enables operations based on PDB file secondary structures (e.g., chains and helixes). | |
| | | Edit=> Point Group | Specify/impose symmetry on the current model. | |
| | Crystal Editor | Edit=>PBC | Create and modify unit cells for periodic structures. | |
| | MO Editor | Edit=>MOs | View, reorder and modify occupancy for molecular orbitals. | |
| | Symmetrize | Edit=>Symmetrize | Apply point group symmetry to the current model. | |
| | | Edit=>Reorient | Restore canonical molecule orientation. | |
| | Rebond | Edit=>Rebond | Recompute the bound atoms, identifying bonded atoms based on a distance algorithm. | |
| | Clean | Edit=>Clean | Adjust molecular geometry according to a set of rules designed to match chemical intuition. | |
| | | Edit=>Mirror Invert | Invert the molecule around the selected atom. | |
| | Add View | View=>Add View | Create a new View window, with an independently adjustable view of the current molecule. | |

| Icon | Name | Menu Path | Purpose | Keystroke |
|---|---|---|---|---|
| | Center | View=>Center | Center molecule in the View window (adjusts size). | |
| | | View=>Builder | Close or reopen the standalone **Builder** palette. | |
| | | View=>Hydrogens | Control the display of hydrogens in View window. | |
| | | View=>Dummies | Control the display of dummy atoms in View window. | |
| | | View=>Labels | If selected, label each atom with its serial number (reflecting its sequence in the list of atoms). | |
| | | View=>Symbols | If selected, display the chemical symbol for each atom. | |
| | | View=>Bonds | Control the display of bonds in the View window. | |
| | | View=>Synchronize | Link views to synchronize mouse-based manipulations. | |
| | | View=> Cartesian Axes | Control the display of X,Y,Z axes in the View window. | |
| | | View=> Stereochemistry | Indicate molecule's stereochemistry by labeling relevant atoms as R or S. | |
| | | View=>Positioning Tools | Display the molecule positioning tools icons in the View window toolbar. | |
| | Display Format | View=> Display Format | Specify the display format for molecules and surfaces. | Ctrl-D |
| | Calculation | Calculate=> Gaussian Calculation Setup | Set up Gaussian input for the molecular structure in the current view winodw and optionally run the job. | Ctrl-G |
| | Quick Launch | Calculate=> Gauss. Quick Launch | Run a Gaussian job for the current molecule, bypassing the **Gaussian Calculation Setup** dialog. | |
| | Schemes | Calculate=> Gauss. Calc. Scheme | Define and modify Gaussian calculation schemes. | |
| | Current Jobs | Calculate=> Current Jobs | Display currently running GaussView-initiated Gaussian jobs (including CubeGen and FreqChk). | Ctrl-J |
| | | Results=> Summary | Provide summary data of the results of a Gaussian calculation (after a results file is opened). | |
| | | Results=>Charge Distribution | Display partial charge density, as computed by various Gaussian methods. | |
| | | Results=> Surfaces/Contours | Create, load, save and display surfaces and contours. | |
| | | Results=> Vibrations | Display calculated vibrational and other spectral data, including normal mode animation. | |
| | | Results=>NMR | Display calculated NMR spectra. | |
| | | Results=>UV-VIS | Display predicted UV/Visible spectra. | |
| | | Results=>Scan | Display plots of potential energy surface scans. | |
| | | Results=>IRC/Path | Display plots of predicted IRC paths. | |
| | | Results=>Trajectory | Display trajectory plots from ADMP or BOMD calculations. | |
| | | Results=> Optimization | Display plots of geometry optimization results. | |
| | View File | Results=>View File | Start an editor session for the log file for the current molecule. | |
| | Stream | Results=>Stream Output File | Display output from a currently running Gaussian calculation continuously as it becomes available. | |

| Icon | Name | Menu Path | Purpose | Keystroke |
|---|---|---|---|---|
| | | Windows=>Molecule Groups=>Show All | Display/restore windows for all model groups. | |
| | | Windows=>Molecule Groups=>Show None | Hide windows for all model groups. | |
| | | Windows=>Molecule Groups=>*name* | Display/restore windows for the specified model group | |
| | | Windows=> Minimize All | Minimize all view windows. | |
| | | Windows=> Restore | Raise active View window. | |
| | | Windows=> Restore All | Open all minimized view windows. | |
| | | Windows=>Close | Close the active View window. | |
| | | Windows=> Close All | Close all open view windows. | |
| ⇦ | Previous | Windows=>Previous | Activate the previous View window in sequence. | PgUp |
| ⇨ | Next | Windows=>Next | Activate the next View window in sequence. | PgDown |
| ❐ | Cascade | Windows=>Cascade | Arrange all view windows in an overlapped pile. | |
| ⊞ | Tile | Windows=>Tile | Resize and rearrange view windows so that all are visible. | |
| | | Windows=>*name* | Make the specified View window the active one. | |
| ? | Help | Help=> GaussView Help | Open the GaussView help facility. | Ctrl-H |
| | | Help=> Gaussian Help | Open the Gaussian website's help section in the default browser. If Internet access is not available, a local copy included within the GaussView application tree is opened instead. | |
| | | Help=> About GaussView | Display the GaussView copyright and version information. | |
| | | Help=> GaussView Tips | Display GaussView tips. | |
| $^{6}\mathrm{C}$ | Elements | | Open the **Element Fragments** palette. | |
| ⬡ | Rings | | Access a palette of ring structures. | |
| -R | R-Group Fragment | | Summon a palette of functional group fragments. | |
| | Biological Fragments | | Summon a palette of amino acid and nucleoside fragments. | |
| | Custom Fragment | | Access a custom fragment library. | |
| ↔ | Modify Bond | | Access **Bond SmartSlide** dialog after two atoms are selected. | |
| ∠ | Modify Angle | | Access **Angle SmartSlide** dialog after three atoms are selected. | |

| Icon | Name | Menu Path | Purpose | Keystroke |
|---|---|---|---|---|
| | Modify Dihedral | | Access **Dihedral SmartSlide** dialog after four atoms are selected. | |
| ? | Inquire | | Examine structural data for the current molecule. | |
| H | Add Valence | | Add an additional hydrogen to the selected atom. | |
| | Delete Atom | | Eliminate atoms and/or open valences (dangling half bonds). | |
| | Invert About Atom | | Invert molecular structure about a selected atom. | |
| | Select by Clicking | | Select atoms by clicking on them. | |
| | Select by Marquee | | Select atoms by clicking and dragging a marquee enclosing them. | |
| | Select None | | Deselect all currently selected atoms. | |
| | Select All | | Select all atoms. | |
| ▸ Builder Fragment: | Fragment Placement | | Open panel containing fragment placement options within the control window. | |
| *Icons found in the Active Model View window:* | | | | |
| | Animate | | Display all models within the molecule group in succession. | |
| | Stop Animation | | Stop an animated display. | |
| | Single View | | Display only one model within the molecule group. | |
| | Multi View | | Display all models within the molecule group. | |
| *Icons found in the five Fragment Palette windows:* | | | | |
| | Tacked | | Keep this palette open until explicitly closed (amodal operation). | |
| | Untacked | | Close palette when a different one is opened (modal operation). | |
| *Icons related to various coordinate editing dialogs:* | | | | |
| Z | Z-matrix Coordinates | | Display Z-matrix coordinates. | |
| C | Cartesian Coordinates | | Display Cartesian coordinates. | |
| F | Fractional Coordinates | | Display fractional coordinates for periodic systems. | |
| L | ONIOM Layers | | Display ONIOM layer assignments and related data. | |
| M | MM Parameters | | Display Molecular Mechanics atoms types and other data. | |
| P | PDB Info | | Display residue and chain assignments from a PDB file. | |

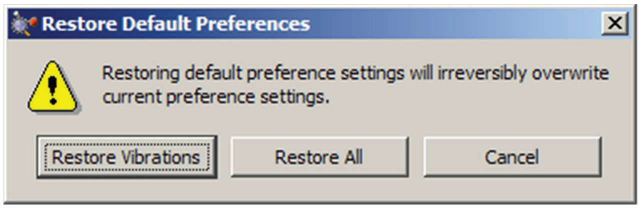
| Icon | Name | Menu Path | Purpose | Keystroke |
|---|---|---|---|---|
|  | **Isotope Masses** |  | Display column(s) containing isotopes mass(es). |  |
|  | **Create a New Coordinate** |  | Add a new redundant coordinate in the **Redundant Coordinate Editor**. |  |
| ⇧ | **Sort Ascending** |  | Sort rows in ascending order in the **Atom List Editor**. |  |
| ⇩ | **Sort Descending** |  | Sort rows in descending order in the **Atom List Editor**. |  |
| *General icons used many places within GaussView:* |  |  |  |  |
| ⇧ | **Move Up** |  | Move the selected item up in a list. |  |
| ⇩ | **Move Down** |  | Move the selected item down in a list. |  |
| > | **Add Selected** |  | Add the selected item to a list. |  |
| >> | **Add All** |  | Add all items to a list. |  |
| < | **Remove Selected** |  | Remove the selected item from a list. |  |
| << | **Remove all** |  | Remove all items from a list. |  |

## GaussView Preferences

Default settings for many GaussView features can be customized via the preferences, which are reached with the **File=>Preferences** menu path. The following preferences are available:

- **Building**: Set default settings for advanced fragment placement options for all three sets (Default, Old and Custom).
- **Charge Distribution**: Specify desired settings for displaying atomic charge and dipole moment data.
- **Clean Controls**: Set the adjustable parameters and controls for the structure cleaning function.
- **Colors**: Customize the coloring of various GaussView displays.
- **Desktop**: Define file associations for extensions associated with Gaussian and GaussView files (Windows version only).
- **Display Format**: Set the preferred **Display Format** dialog settings for view windows.
- **File/Directory**: Set preferred directory locations for various GaussView contexts.
- **Gaussian Setup**: Set the preferred **Gaussian Calculation Setup** dialog settings.
- **Icons**: Set default icon sizes in the user interface.
- **Image**: Set the preferred values for capturing images.
- **Job Setup**: Define execution procedures for Gaussian and related jobs.
- **Movie**: Specify preferences for animations created by GaussView.
- **Print**: Set the preferred values for printing images.
- **Vibrations**: Set the preferred **Display Vibrations** dialog settings.
- **Window Behavior**: Set the preferred behavior for dialogs.

All of the preferences dialogs contain several buttons: **Ok** (save current settings and exit), **Cancel** (exit and discard unsaved changes), **Default** (restore GaussView's installation settings) and **Help** (obtain online help). When you use the **Default** button, the dialog in Figure 7 will appear.


Restore Default Preferences
Restore Vibrations
Restore All
Cancel

Restoring default preference settings will irreversibly overwrite current preference settings.

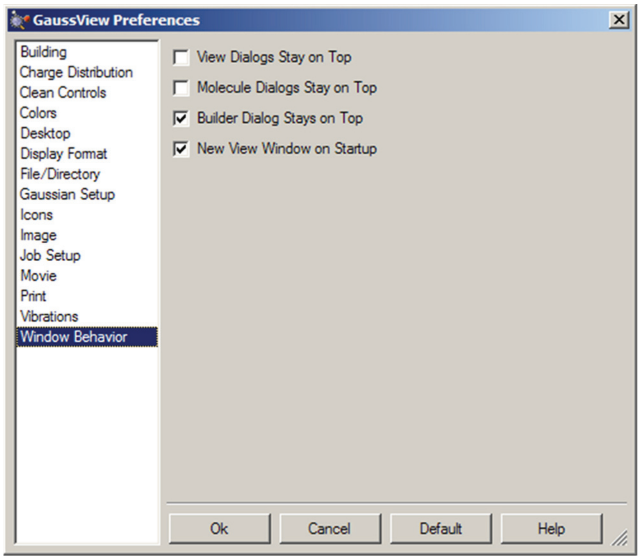
Figure 7. Restoring Default Preferences

*When you click the Default button in the Preferences, you are given the choice of restoring all default preferences or only the ones pertaining to the current dialog (here, the default preferences for Vibrations).*

We will consider two of the preferences next. The others will be discussed along with the relevant features in the course of this manual.

## Specifying GaussView Window Behavior

The **Window Behavior Preferences**, illustrated in Figure 8, controls how various GaussView window types behave.


GaussView Preferences
Building
Charge Distribution
Clean Controls
Colors
Desktop
Display Format
File/Directory
Gaussian Setup
Icons
Image
Job Setup
Movie
Print
Vibrations
Window Behavior
Ok
Cancel
Default
Help

☐ View Dialogs Stay on Top
☐ Molecule Dialogs Stay on Top
☑ Builder Dialog Stays on Top
☑ New View Window on Startup

Figure 8. Window Behavior Preferences

*These settings allow you to force certain window types to remain uppermost, as well as whether an empty View window is automatically created when the program starts.*

## Modifying Icon Sizes

The **Icons Preferences** allow you to specify the icon sizes for various GaussView windows and toolbars. It is illustrated in Figure 9. The controls in the dialog control the icons for menus, toolbars and the standalone **Builder** palette. The defaults are small icons for the first two items and large icons for the third one.

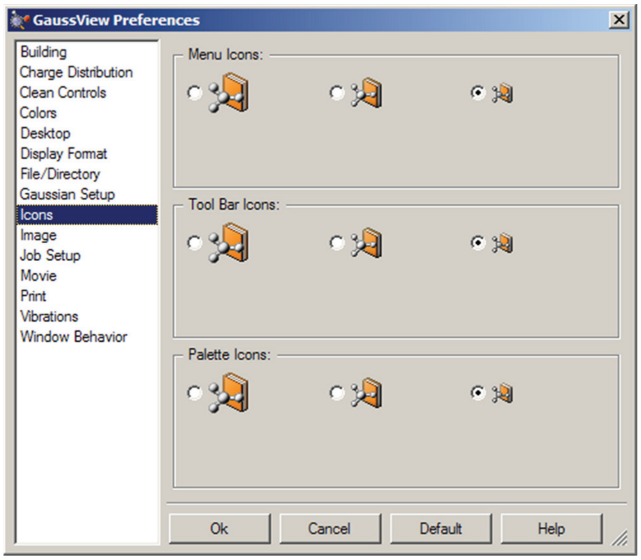
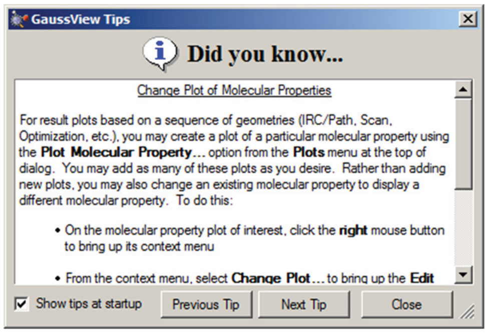

GaussView Preferences
Building
Charge Distribution
Clean Controls
Colors
Desktop
Display Format
File/Directory
Gaussian Setup
Icons
Image
Job Setup
Movie
Print
Vibrations
Window Behavior
Menu Icons:
○ ○ ●
Tool Bar Icons:
○ ○ ●
Palette Icons:
○ ○ ●
Ok
Cancel
Default
Help

**Figure 9.** Customizing Icon Sizes
*You can select larger icons for various GaussView windows with this preference.*

## Displaying GaussView Tips

The **Help=>GaussView Tips** menu path opens the **GaussView Tips** window, which displays various tips for using the program effectively. You can also choose to have a tip displayed each time GaussView starts up using the checkbox at the bottom of the window (the default is unchecked).


GaussView Tips
Did you know...

Change Plot of Molecular Properties

For result plots based on a sequence of geometries (IRC/Path, Scan, Optimization, etc.), you may create a plot of a particular molecular property using the **Plot Molecular Property**... option from the **Plots** menu at the top of dialog. You may add as many of these plots as you desire. Rather than adding new plots, you may also change an existing molecular property to display a different molecular property. To do this:

- On the molecular property plot of interest, click the **right** mouse button to bring up its context menu
- From the context menu, select **Change Plot**... to bring up the **Edit**

☑ Show tips at startup

Previous Tip
Next Tip
Close

**Figure 10.** GaussView Tips
*Click Show tips at startup to view a tip each time you start GaussView.*

# Building Molecules

This section describes GaussView's molecule building features. These options enable you not only to construct new structures either atom-by-atom or from fragments, but also to manipulate and examine previously-computed molecules. See the next major section of this manual, "Opening, Displaying and Saving Molecules and Views," for information on using GaussView view features and opening and saving molecule files and images.

## Placing Elements and Fragments

The GaussView molecule building tools always operate on the active View window. In general, GaussView begins and remains in its insert/replace mode, unless one of the options described below explicitly calls for it to act in a different manner. Clicking in an open area of the View window adds the current atom or fragment to the window as a distinct fragment. Clicking on an existing atom adds the current item to the existing structure at the indicated point, usually replacing it (other options are discussed later).

The desired atom or fragment is chosen using one of the **Element**, **Functional Groups**, **Rings** and **Biological Fragments** buttons and then selecting one of the choices from the resulting palette. The current item always appears in the **Current Fragment** area of the GaussView control window and/or the **Active Fragment** area of the standalone **Builder** palette (see Figure 3). Clicking on either the **Active Fragment** area on the standalone **Builder** palette or on the fragment name above the main window's **Current Fragment** area opens the palette corresponding to the selected fragment type.

Note that the standalone **Builder** palette is opened with the **View=>Builder** menu item and can be made to always stay on top of all other open windows by checking the **Builder Dialog Stays on Top** checkbox in the **Window Behavior Preferences** (accessed with the **File=>Preferences** menu path).

### The Element Fragments Palette

The **Element Fragments** palette allows you to select an element from the periodic table. The various possible coordination patterns for the selected element are shown at the bottom of the window (see Figure 11). The default element type is tetrahedral carbon.

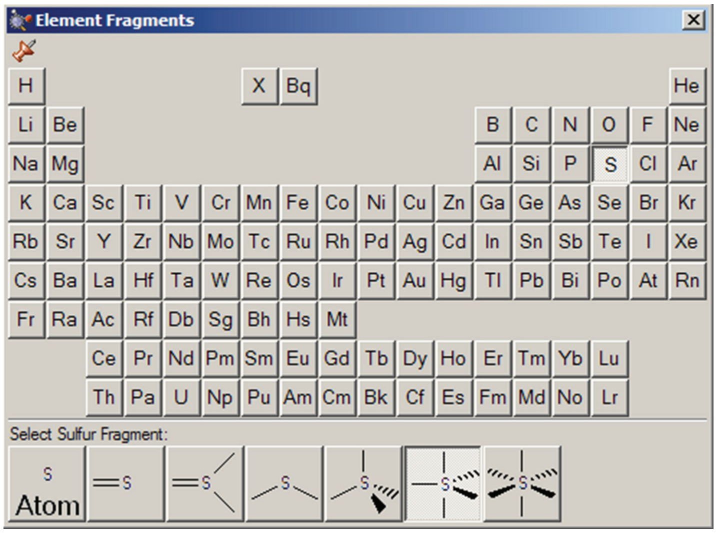

Element Fragments
H
X Bq
He
Li Be
B C N O F Ne
Na Mg
Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Ac Rf Db Sg Bh Hs Mt
Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
Th Pa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

**Figure 11.** The Element Fragments Palette

*The available hybridization (connectivity) variations for the selected element appear along the bottom of the palette. In this case, the current atom type is pentavalent sulfur.*

## The R-Group Fragments Palette

The **R-Group Fragments** window allows you to select from a series of AM1-optimized functional group fragments. It is illustrated in Figure 11. The default group is carbonyl (formaldehyde).

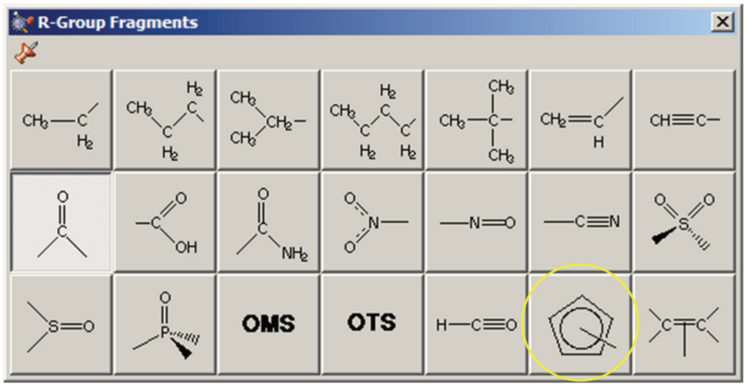


**Figure 12.** The R-Group Fragments Palette
*Use this palette to select the desired functional group.*

Note that several of the fragments use non-traditional bonding. These fragments include a five-member ring with an open bond perpendicular to the plane of the ring: a $n^5$-cyclopentadienyl ligand for use in constructing organometallic systems (circled in Figure 12).

## The Rings Palette

The Ring Fragments window allows you to select from a series of AM1-optimized ring structures. It is illustrated in Figure 13. The default ring is benzene.

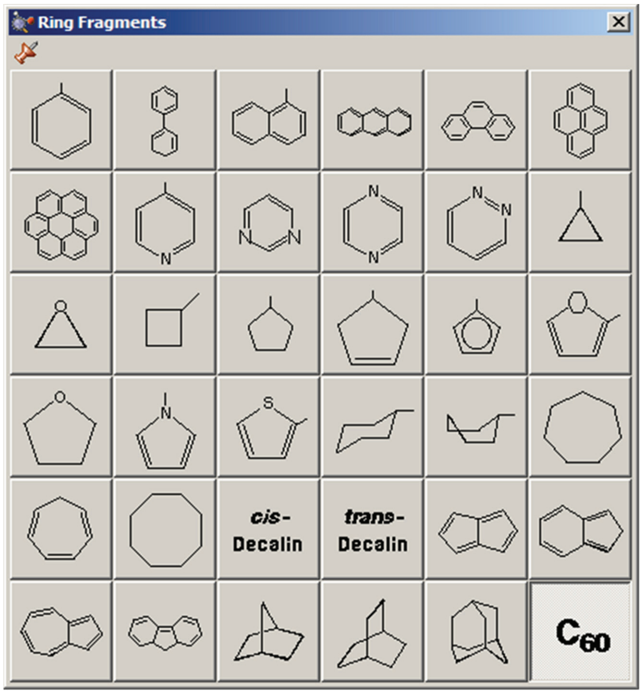
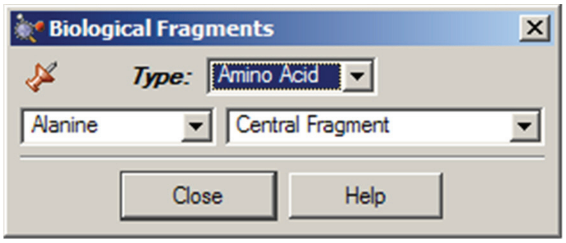


**Figure 13.** The Ring Fragments Palette
*Use this palette to select the desired ring system.*

## The Biological Fragments Palette

The **Biological Fragments** palette presents a set of AM1-preoptimized fragments useful to biological researchers: the amino acids and various DNA bases (see Figure 13). The default biological fragment is Alanine Central Residue.



Type: Amino Acid

Alanine

Central Fragment

Figure 14. Selecting Biological Fragments

*Use the various fields in this window to select amino acids and DNA bases.*

The **Type** field allows you to select either **Amino Acid** or **Nucleoside**. When **Amino Acid** is selected, the left popup menu below the **Type** field can be used to select the desired amino acid, and the right popup menu in that line allows you to specify the structural form as **Central Fragment**, **Amino-Terminal Fragment** or **Carboxyl-Terminal Fragment** (the last two are the N-terminated and C-terminated forms, respectively).

When the **Type** field is set to **Nucleoside**, the left popup menu below the **Type** field can be used to select the desired DNA base (nucleic acid fragment), and the right popup menu in that line allows you to specify the structural form as **Central Fragment**, **C3'-Terminal Fragment**, **C5'-Terminal Fragment** or **Free Nucleoside**.

### Making Palettes Sticky

The various palettes in GaussView can be used in a modal (dialog box behavior) or amodal (floating palette behavior) manner. The thumbtack icon in the upper left corner of the window shows whether the palette will close when another one is selected (or a non-building context is entered). The green pushed-in tack indicates that the palette is "tacked" to the desktop (i.e., "sticky"): 📌 ; the red upward pointing tack similarly indicates modal operation: 📌 .

## Placing a Fragment in a Centroid Position

The **Place Fragment at Centroid of Selected Atoms** item on the **Builder** context menu (reached by right clicking in an open area of a View window) will place the current element, R-group, ring or biological fragment at the centroid position defined by the currently selected atoms. For example, to place an atom inside a $C_{60}$ cage, select all of the atoms in the molecule, select the desired atom from the **Element Fragments** palette (specifying the bare atom type), right click in an open area of the view, and select **Builder=>Place Fragment at Centroid of Selected Atoms**. This process is illustrated in Figure 15.

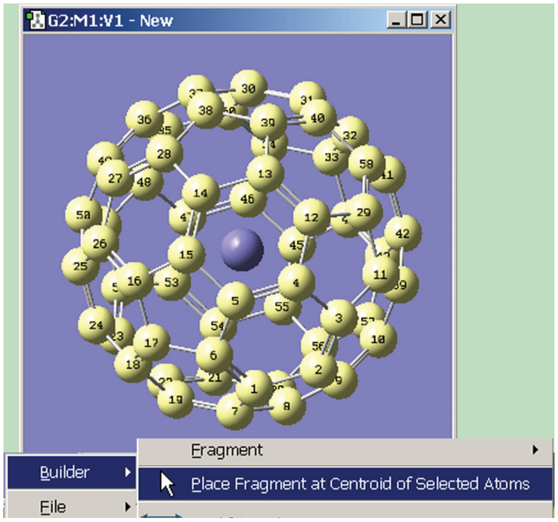


Figure 15. Placing a Centroid Atom in $C_{60}$

Note that if you simply want to define the centroid location without immediately placing any atoms there, you can use the dummy atom (element type **X**) to do so.

Atom selection methods are discussed in detail in a later section below.

### Undo and Redo

The **Edit=>Undo** and **Edit=>Redo** menu paths may be used to reverse or reinstate a previous molecule modification or other action. The **Undo** button and the **Redo** button may be used for the same purposes.

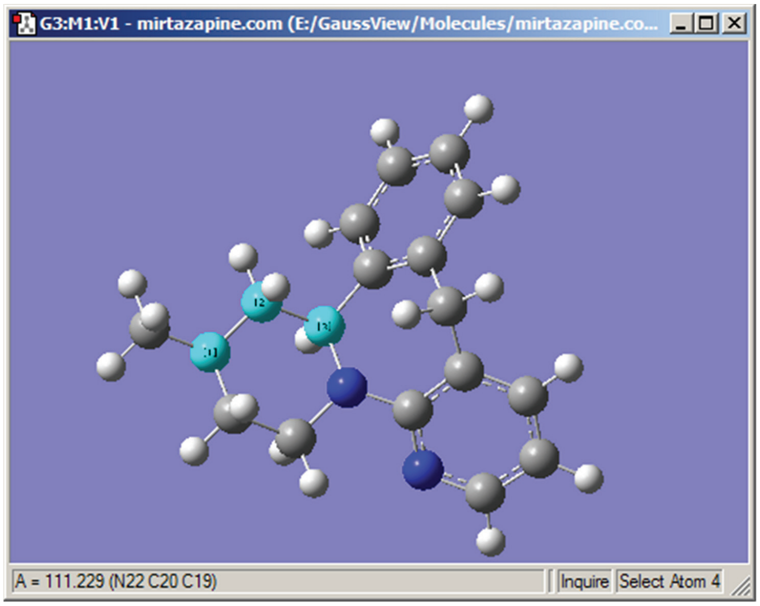
## Viewing and Adjusting Structure Parameters

The Builder toolbar/window includes the following buttons for viewing and modifying the structural parameters of molecules: **Bond**, **Angle**, **Dihedral**, **Inquire**, **Add Valence**, **Delete Atom**, and **Invert About Atom**. In addition, other buttons and their corresponding menu items also affect molecular structure—including **Clean**, **Rebond**, and **Symmetrize**—and display. We will consider these features in this section.

### Inquire Mode

The **Inquire** button allows you to request geometric information directly from the View window when you click on the atoms of interest. Note that the selected atoms do not need to be bonded. The structural information appears in the View window's status bar, as in Figure 14. The number of atoms that you select affects the resulting display on the View window:

- Hover over atom: atom type and number: Atom 22(N).
- 1 atom: Atom type and number: N22.
- 2 atoms: Bond length (distance): B = 1.45768 (N22 C20).
- 3 atoms: Interatomic angle: A = 111.229 (N22 C20 C19).
- 4 atoms: The 4-3-2-1 dihedral angle: D = -58.360 (N22 C20 C19 N21).


G3:M1:V1 - mirtazapine.com (E:/GaussView/Molecules/mirtazapine.co...

A = 111.229 (N22 C20 C19)

**Figure 16.** Inquire Mode Display

*This display shows the value of the selected bond angle in the window's lower left corner.*

## Semichem SmartSlides

Three buttons, the **Bond** button, the **Angle** button, and the **Dihedral** button, allow rapid and intuitive modification of geometric components. Once selected, the atoms of the bond in question must be selected for the respective SmartSlide dialog box to open. Once you have modified a parameter using the SmartSlide, the **OK** button must be pressed before any of the changes made on any SmartSlide are actually applied to the molecule. Clicking the close box will discard any changes (as will selecting the **Cancel** button).

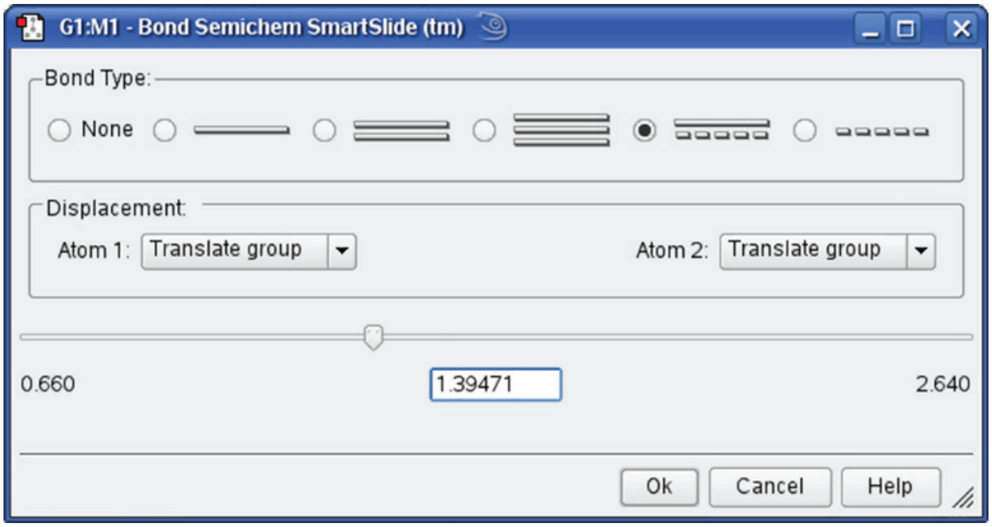
### The Bond SmartSlide

The **Bond SmartSlide** is illustrated in Figure 17. The initial bond length value is set to the distance between the selected pair of atoms, and the type of bond existing between them is indicated. The SmartSlide provides access to all the possible bond types.

The interatomic distance is dynamically adjusted by moving the slider along the scale. Values may also be directly entered in the text box.

You can change the bond type by clicking one of the bond type radio buttons without affecting the valence on the atoms from which the bonds are removed.

Note that the **Bond SmartSlide** is also used to add bonds between unbonded atoms. Simply click on the two atoms to be bonded as usual. When the SmartSlide opens, click on the type of bond desired, and the bond will be created. Similarly, to remove a bond, select the two atoms you want to unbond, and then select the **None** radio button in the dialog.



● (selected bond type)

Atom 1: Translate group

Atom 2: Translate group

0.660

1.39471

2.640

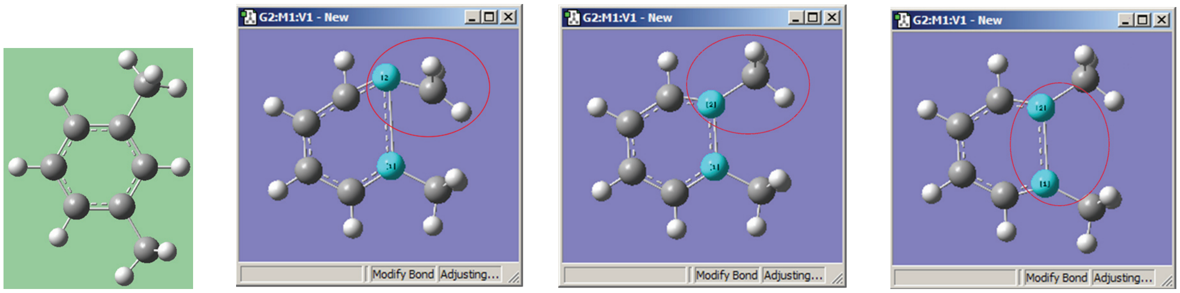
Figure 17. The Bond SmartSlide

*This dialog can be used to add, remove and change bond lengths.*

The **Displacement** fields specify how attached groups are handled as the bond distance changes:

- **Translate Atom**: Move only the atom, keeping the group's position fixed in space.
- **Translate Group**: Move the attached group along with the atom (i.e., as a single unit).
- **Fixed**: Do not allow the atom or the group to move (all movement occurs at the other atom).

Figure 18 illustrates the effects of different combinations of these choices.



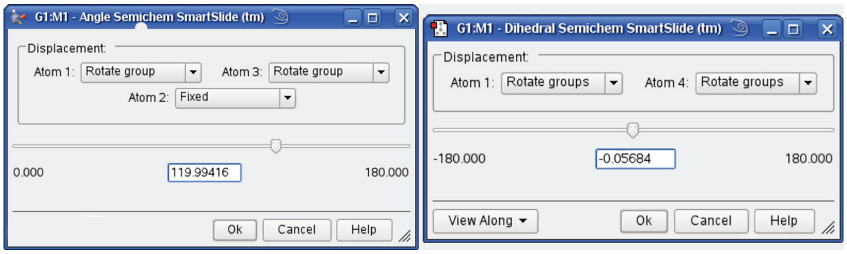
Original 1=Fixed, 2=Translate Atom 1=Fixed, 2=Translate Group 1,2=Translate Group

**Figure 18.** Bond Length Modification Options

*All three of these structures result from lengthening the bond distance between the two selected C atoms (to the same value in all three cases). In the left picture, atom 1 was held fixed, and atom 2 was set to Translate Atom. Compare this to the middle picture which also held atom 1 fixed and set atom 2 to Translate Group. The upper methyl group stays fixed in the first case, while the 1-2-R bond angle remains unchanged in the center case. The right picture sets both atoms to Translate Group, probably the most common choice for a case like this one.*

### The Angle and Dihedral SmartSlides

Figure 19 illustrates the dialog associated with the **Angle SmartSlide**. The dialog for the **Dihedral SmartSlide** is similar, but it includes **Displacement** fields only for Atom 1 and Atom 4.


G1:M1 - Angle Semichem SmartSlide (tm)

Displacement:
Atom 1: Rotate group
Atom 3: Rotate group
Atom 2: Fixed

0.000 119.99416 180.000

G1:M1 - Dihedral Semichem SmartSlide (tm)

Displacement:
Atom 1: Rotate groups
Atom 4: Rotate groups

-180.000 -0.05684 180.000

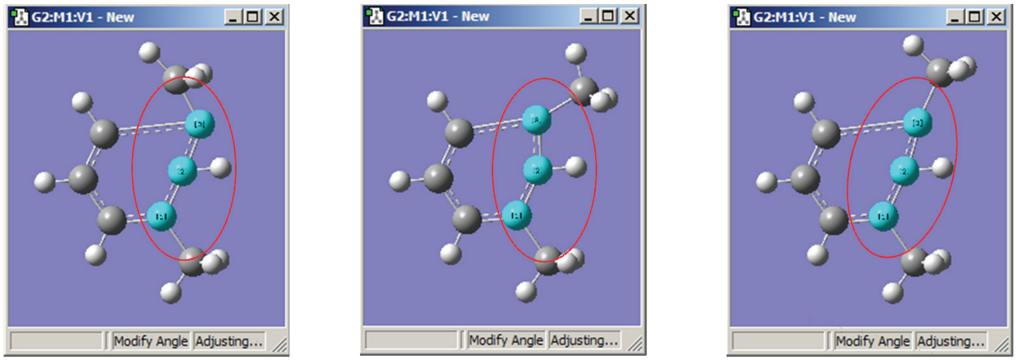
**Figure 19.** Angle and Dihedral SmartSlides

*These dialogs modify bond angles and dihedral angles.*

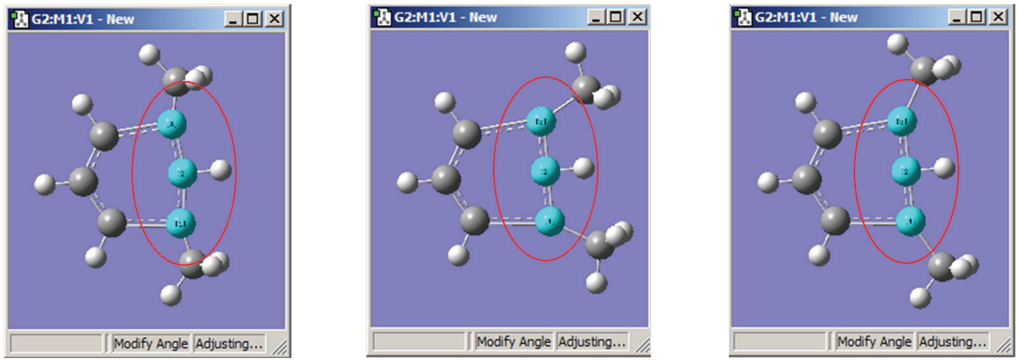
Figure 20 illustrates some of the combinations of various **Displacement** settings for bond angles (using the same original molecule as Figure 18). The possible choices are:

- **Rotate Atom**: Move only the atom, keeping the group's position fixed in space.
- **Translate Group**: Move the attached group along with the atom as a single unit.
- **Rotate Group**: The group's position rotates along with the atoms as the angle changes.
- **Fixed**: Do not allow the atom or the group to move (all movement occurs at other atoms).

The **View Along** popup menu in the lower left corner of the **Dihedral SmartSlide** dialog allows you to reposition the molecule using a Newman projection, along the 2,3 internuclear axis or the 3,2 internuclear axis.



1,2=Fixed, 3=Rotate Atom 1,2=Fixed, 3=Rotate Group 1,2=Fixed, 3=Translate Group



1,3=Rotate Atom, 2=Fixed 1,3=Rotate Group, 2=Fixed 1,3=Translate Group, 2=Fixed

**Figure 20.** Bond Angle Modification Options

*All six of these structures result from increasing the 1-2-3 bond angle. In the top row, atoms 1 and 2 are both held fixed. Compare the results of increasing the bond angle to the same value in the three cases (keeping in mind the "normal" position for the ring atoms and the methyl groups). The movement of the methyl group attached to atom 3 ranges from substantial in the first frame to a little in frame 2 to almost none in frame 3. In the second row, atom 2 is held fixed while other choices are used for atoms 1 and 3. Comparison of these illustrations as well as experimentation will make the differences between the choices clear and familiar.*

## Adding and Deleting Valences

The **Add Valence** button attaches additional valences (shown as hydrogen atoms) to the center clicked with the mouse. The new valences will be placed as far as possible from the other atoms attached to the center.

Similarly, the **Delete Atom** button removes atoms and open valences. When used, the function will eliminate the selected atom and all single valences (hydrogens) attached to it. It may also be used to remove a dangling bond by clicking on the bond stick (see Figure 21).

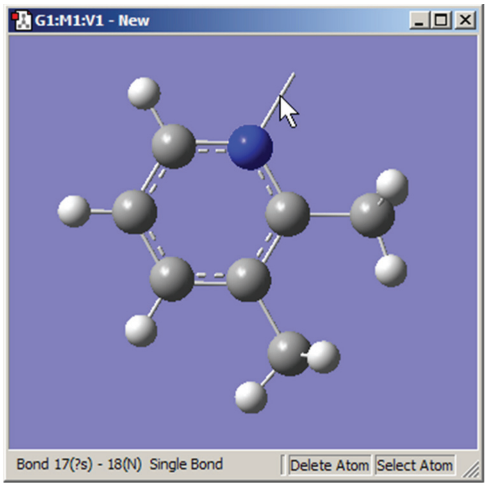

G1:M1:V1 - New
Bond 17(?s) - 18(N) Single Bond
Delete Atom
Select Atom

**Figure 21.** Deleting a Dangling Bond (Open Valence)
*The Delete Atom button may be used to remove atoms and dangling bonds. An example of the latter is shown at the top of the molecule. Clicking on it will remove the open valence.*

## Invert About Atom (Mirror Invert)

The **Invert About Atom** button allows you to reverse the symmetry of a molecule with respect to a selected atom. Figure 22 illustrates the use of this feature.

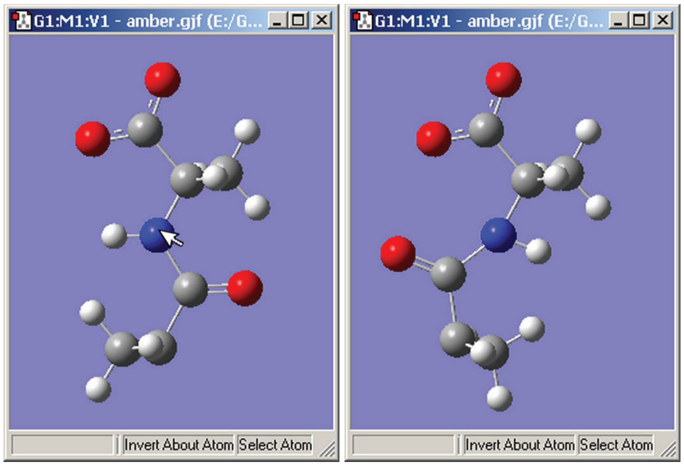
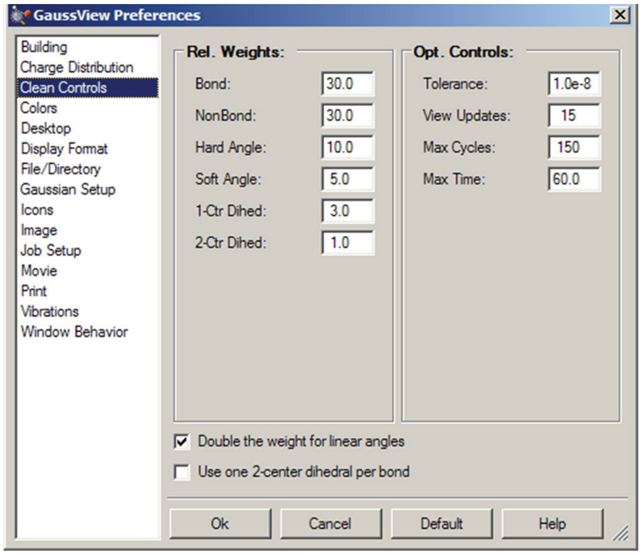

G1:M1:V1 - amber.gjf (E:/G...
Invert About Atom
Select Atom
G1:M1:V1 - amber.gjf (E:/G...
Invert About Atom
Select Atom

**Figure 22.** Inverting a Structure About an Atom
*Clicking on the nitrogen atom with the Invert About Atom tool will result in the structure on the right.*

## Cleaning Structures

The **Clean** button and **Edit=>Clean** menu items both adjust the geometry of the molecule, based on a defined set of rules, to more closely match chemical intuition. The results are only approximations and are not intended to be perfect. Geometries may require adjustment for non-classical cases such as transition states.

The GaussView clean function may be customized via the **Clean Controls Preferences** panel (illustrated in Figure 23).



Rel. Weights:
Bond: 30.0
NonBond: 30.0
Hard Angle: 10.0
Soft Angle: 5.0
1-Ctr Dihed: 3.0
2-Ctr Dihed: 1.0

Opt. Controls:
Tolerance: 1.0e-8
View Updates: 15
Max Cycles: 150
Max Time: 60.0

☑ Double the weight for linear angles
☐ Use one 2-center dihedral per bond

Figure 23. Customizing the Clean Function

*You can use this preference panel to modify and customize how the GaussView clean function operates.*

The default clean settings attempt to achieve a balance that produces expected "normal" results. Altering the settings in **Clean Controls Preferences** can cause unexpected and undesirable results, so please read the following sections carefully before making any changes.

The following controls are available in the dialog. The fields in the **Rel. Weights** column are:

- **Bond**: The targeted bond lengths are assigned based on the van der Waals radii of the two atoms forming the bond, with slight adjustment for bond type. They are not intended to be chemically accurate, but they should give reasonable input geometries for Gaussian.
- **NonBond**: Repulsive term between all atoms that are not directly bonded. The purpose of this component is to keep atom centers apart so one atom is never masking another atom. However, it will not adjust biphenyl.
- **Hard Angle**: Hard angles are calculated for atom centers that contain 2-4 bonds. They are weighted more heavily since the targeted angles are known. These terms are vital for maintaining atom center integrity.
- **Soft Angle**: Soft angles are calculated for atom centers that contain 5 or more bonds. The targeted angles are not well known, but desired results can be achieved with practice. To produce a trigonal bipyramidal structure, adjust the axial bond angle to 180 degrees. Make sure the linear angle bias option is on. Most of the time, the clean procedure will produce the desired structure. Practice with coordinate patterns to get a feel for cleaning more complex coordinations.
- **1-Ctr Dihed**: Calculated from the Newman projections down each bond and limited to atom centers with less than 5 bonds. This term helps maintain atom center integrity when the 2-center dihedrals are causing distortions.
- **2-Ctr Dihed**: This is the only term that affects tertiary structure. The targeted dihedrals will be eclipsed or staggered based on the bond types. If each atom center contains multiple bonds, the targeted dihedral will be eclipsed.

The checkboxes at the bottom of the window have the following effects:

- **Double the weight for linear angles**: This term assists cleaning with soft angles where the angles at an atom center are not well known.
- **Use one 2-center dihedral per bond**: Normally, this option should remain unchecked. It is available to provide better performance on slower systems.

The fields in the **Opt. Controls** column are:

- **Tolerance**: Lower values give more accurate structures, but can take significantly longer to clean. The range should be between 1.0E-5 and 1.0E-12.
- **View Updates**: Controls how often the views of the molecule being cleaned are updated. A value of 1 gives a refresh with every clean cycle. A value of 10 gives a refresh every 10 clean cycles. A value of 0 disables view updates until clean is complete. Depending on your system, this parameter can have a significant effect on cleaning time.
- **Max Cycles**: Maximum number of steps during a clean optimization. A good value is 150. Larger structures may require a larger value.
- **Max Time**: Maximum time (seconds) allowed for a clean operation to complete.

It is important to remember that the various components of the clean force field are relative. Changing one weight will affect the behavior of the other weights. For example, an excessive non-bond weight will produce longer bonds. Similarly, an excessive hard angle weight could affect the 2-center dihedrals.

You can disable any set of terms by assigning a weight of 0.0. For example, disabling the 1-center dihedral term can result in faster cleaning, but the resulting tertiary structure may not be as nice. Do not disable the bond weight or hard angle terms. The former should be kept high relative to the other terms.

### Clean Performance Tips

If the clean function is too slow on your system, try these settings:

- **NonBond**: 0
- **1-Ctr Dihed**: 0
- **Use one 2-center dihedral per bond**: checked
- **View Updates**: 0

Poor performance of the clean function can also be a symptom of a memory shortage on the system.

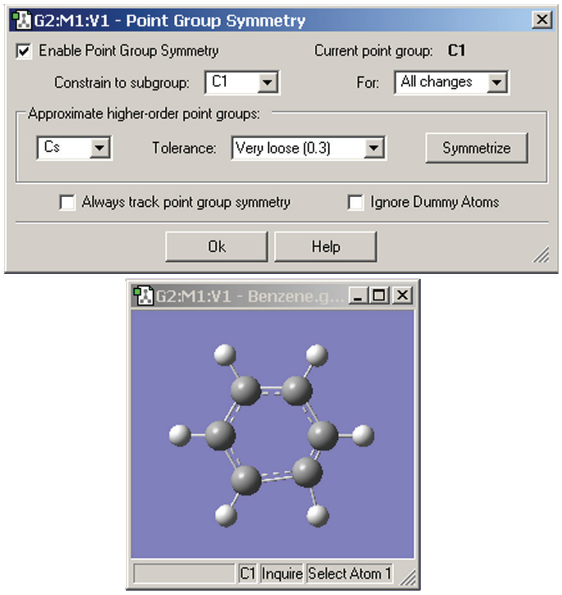
## Rebonding Structures

The **Rebond** button and **Edit=>Rebond** menu path both initiate a rebonding process in which GaussView reidentifies bonded atoms, based on a distance algorithm. Note that Gaussian usually does not use the bond information on the screen for calculations. This information is presented primarily to make it convenient for you to visualize the chemistry of the molecule.

## Imposing Symmetry

The **Point Group Symmetry** dialog is used to specify the desired symmetry for a molecular structure (see Figure 24). It is reached via the **Edit=>Point Group** menu path. The controls have the following meanings:

- **Enable point group symmetry**: Enable GaussView's symmetry features.
- **Constrain to subgroup**: Select a point group to which to constrain the structure.
- **For**: Select **All changes** to impose symmetry on future structural changes. **None** disables symmetry constrains.
- **Approximate higher-order point groups**: Higher symmetry subgroups which might apply.
- **Tolerance**: Cutoff level below which to consider structural parameters equal.
- **Symmetrize button**: Impose the selected higher-order point group on the molecular structure immediately.
- **Always track point group symmetry**: Tells GaussView to continuously compute point group assignments as the geometry changes. Use this item in conjunction with a symmetry constraint setting of **None** in order to view point group changes continuously as you adjust structural parameters (e.g., use the bond length slider). Normally, the point group is identified only after the change is completed. For very large molecules on slower systems, enabling this item may cause noticeable delays in response time.



G2:M1:V1 - Point Group Symmetry

☑ Enable Point Group Symmetry    Current point group: **C1**

Constrain to subgroup: C1    For: All changes

Approximate higher-order point groups:

Cs    Tolerance: Very loose (0.3)

☐ Always track point group symmetry    ☐ Ignore Dummy Atoms

Figure 24. Imposing Symmetry on a Molecular Structure

*In this example, GaussView has identified the current point group of this distorted benzene molecule as C1. It also recognizes that the C2v point group might also be appropriate. Clicking the Symmetrize button will apply the specified point group to the structure. The Tolerance field can be used to tighten or relax the symmetry identification process. In this case, loosening the tolerance allows GaussView to identify the highest applicable point group as D6h.*

The **Symmetrize** button (on the toolbar) and the **Edit=>Symmetrize** menu item both immediately impose the maximum identifiable point group on the current structure, using the most recent **Tolerance** setting from the **Point Group Symmetry** dialog for this molecule (or the default of **Normal**). They also have the side effect of enabling point group symmetry for the molecule (again, using the previous settings, if any).

The View window status bar will indicate any identified and constrained symmetry for the molecule, as illustrated in Figure 23.

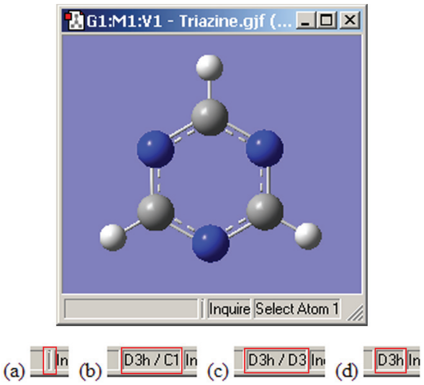


Figure 25. Symmetry-Related Status Bar Displays

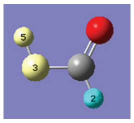
*Four views of the symmetry information section of the status bar for the triazine molecule: (a) symmetry has not been turned on; (b) molecule symmetry (D3h) but no symmetry constraint (C1); (c) molecule symmetry (D3h) and structure constrained to D3 symmetry; and (d) molecule symmetry and constraint symmetry are both D3h.*

## All About Selections: From Atoms to Fragments, Residues, Chains and Beyond

GaussView has a wide variety of different methods and techniques for selecting atoms within molecular structures. Groups of selected atoms are used for many purposes in building structures and setting up Gaussian jobs. This section will discuss the various alternatives, which are summarized in the following list:

- Selection-related toolbar icons: **Select by Clicking**, **Select by Marquee**, **Select All** and **Select None**
- View window selection keystrokes
- Selecting with the **Atom List Editor**, the **PDB Residue Editor**, and the **PDB Secondary Structures Editor**
- Using the **Atom Group Editor**
- The **Atom Selection Editor**

### Selection-Related Toolbar Icons



The main window builder toolbar and the standalone **Builder** palette both contain icons which control item selection behavior and place the cursor in a dedicated selection mode. The icon on the left sets the selection mode to clicking: clicking on an atom toggles its selection mode. Selected atoms appear light yellow (see the two leftmost atoms in the illustration at the right), and their serial numbers are displayed. Contrast this to highlighting where atoms are displayed in light blue for easy identification and/or location (e.g., the hydrogen atom at the lower right). If an atom is both selected and highlighted, it appears light blue (highlighted).

The other selection mode is marquee mode, also called rubberband mode (the icon on the right at the head of this paragraph). In this mode, pressing and holding the mouse button while dragging the cursor will draw a rectangle in the view. When the mouse button is released, all atoms within the defined area are added to the selection. Variations to this default functioning for both modes are available via the **Atom Selection** dialog discussed below.

The other two selection-related icons are the **Select All** and **Select None** buttons, which select and deselect all atoms in the molecule, respectively.

#### Selection Keystrokes in View Windows

These same selection options are available at all times in any View window via the following keystrokes, regardless of the current toolbar icon selection:

| Key | Effect |
|---|---|
| a | Select all atoms. |
| n | Deselect all atoms (select no atoms). |
| r | Marquee selection is active while the R key is held down. |
| c | Individual atom click mode selection is active while the C key is held down. |

### Selecting with the Atom List Editor and Similar Tools

The **Atom List Editor** is discussed in more detail in the next section of this book, but a mention of its selection facilities are relevant here. This dialog, illustrated in Figure 29, provides a spreadsheet-like mechanism for viewing and modifying molecular structures and parameters. The same facilities are also provided by the **PDB Residue Editor** and **PDB Secondary Structure Editor**. There are three main features:

- All of these tools have the ability to highlight various parts/substructures of the molecule, controlled via the **Highlight** column. Highlighted atoms can be selected and deselected via the **Select/Deselect Highlighted Atoms** items on the **View** menu in the Atom List Editor and the similar **Select/Deselect Highlighted Residues** and **Select/Deselect Highlighted Secondary Structures** items in the **View** menus of the other tools.

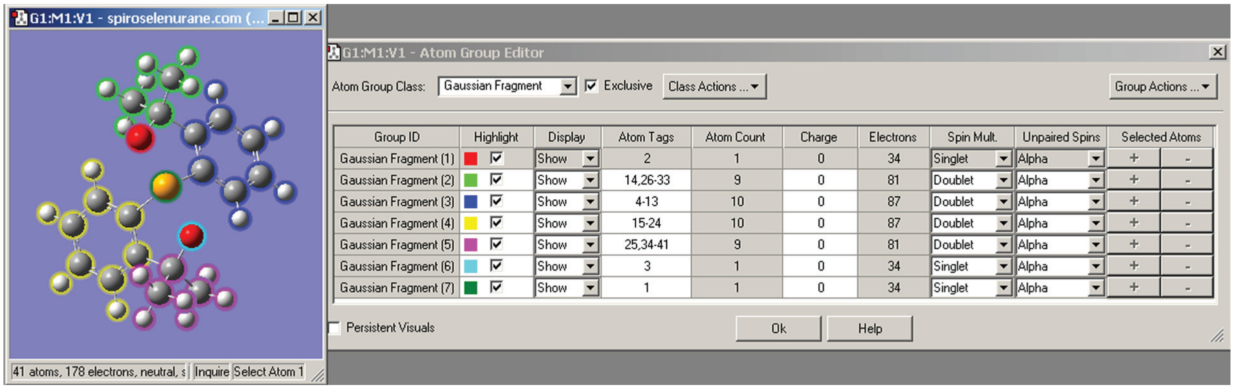
- The **Rows** menus of these three tools all contain the **Select Atoms of Selected Rows** item. Choosing it will cause all atoms corresponding to selected rows in the spreadsheet to be added to the current selection.

- The **Invert Selection** and **Select All** items on the **Rows** menus modify the selection to include all unselected atoms and to include all atoms, respectively.

Somewhat similar functionality is also present in the **ONIOM Layer Editor** discussed later, although this facility's purpose is substantially more specialized.

## Using the Atom Group Editor

The **Atom Group Editor**, reached via the **Atoms Groups** item on the main **Edit** menu, allows you to define subgroups of atoms within a structure for various purposes. It is illustrated in Figure 26.


G1:M1:V1 - spiroselenurane.com (...
41 atoms, 178 electrons, neutral, s
Inquire
Select Atom 1
G1:M1:V1 - Atom Group Editor
Class Actions ...
Group Actions ...
Ok
Help

Atom Group Class: Gaussian Fragment ☑ Exclusive

| Group ID | Highlight | Display | Atom Tags | Atom Count | Charge | Electrons | Spin Mult. | Unpaired Spins | Selected Atoms | |
|---|---|---|---|---|---|---|---|---|---|---|
| Gaussian Fragment (1) | 🟥 ☑ | Show | 2 | 1 | 0 | 34 | Singlet | Alpha | + | - |
| Gaussian Fragment (2) | 🟩 ☑ | Show | 14,26-33 | 9 | 0 | 81 | Doublet | Alpha | + | - |
| Gaussian Fragment (3) | 🟦 ☑ | Show | 4-13 | 10 | 0 | 87 | Doublet | Alpha | + | - |
| Gaussian Fragment (4) | 🟨 ☑ | Show | 15-24 | 10 | 0 | 87 | Doublet | Alpha | + | - |
| Gaussian Fragment (5) | 🟪 ☑ | Show | 25,34-41 | 9 | 0 | 81 | Doublet | Alpha | + | - |
| Gaussian Fragment (6) | 🟦 ☑ | Show | 3 | 1 | 0 | 34 | Singlet | Alpha | + | - |
| Gaussian Fragment (7) | 🟩 ☑ | Show | 1 | 1 | 0 | 34 | Singlet | Alpha | + | - |

☐ Persistent Visuals

**Figure 26.** The Atom Group Editor

*This dialog is used to define fragments and other atoms groups for various types of Gaussian jobs. A separate charge and spin can be optionally assigned to each fragment (as we are doing here). The Atom Group Class popup lists the various kinds of atom groups for which GaussView provides special handling. The Persistent Visuals causes the settings of the Highlight and Display columns to continue to be honored in the View window even after the dialog is closed.*

The various columns in the spreadsheet hold the following data. **Group ID** holds a name for each atom group, typically the class names with a number. When the checkbox in the **Highlight** column is checked, the atoms in the corresponding group are encircled with the indicated highlight color. The menus in the **Display** column allows you to hide the atoms belonging to one or more groups. The **Atom Tags** field lists the serial numbers of the atoms in each group. You can define groups by entering atom numbers here directly, and the field is also updated when atoms are added to or removed from groups by other methods. The **Atom Count** column lists the number of atoms in the group and the **Electrons** column lists the number of electrons (both are read-only). The **Charge**, **Spin Mult** and **Unpaired Spins** columns may be used to set per-fragment charges and spin multiplicities (an example is described later). Finally, the plus and minus sign buttons in each row may be used to add or remove all currently selected atoms from the corresponding group.

Once atom groups are defined, the **Select Atoms** and **Deselect Atoms** items on the **Group Actions** menu can be used to select/deselect atoms within an atom group. The other items on this menu have the following uses:

- **New Group**: Add another group of the current group class. For example, selecting this item in Figure 26 will add another Gaussian Fragment group.
- **Remove** "*item*": Removes the selected atom group. Any atoms in the group are assigned to the first group.
- **Add Selected Atoms to**/**Remove Selected Atoms from**: Equivalent to the plus and minus buttons in the **Selected Atoms** column.

Note that this dialog serves to assign atoms to named groups. None of the items here have any effect on the structure or ever remove any atoms from the molecule.

The defined classes of atom groups are as follows:

| Class | Purpose | Gaussian Calculation Setup Use |
|---|---|---|
| **Gaussian Fragment** | Define atom fragments for use in molecule specifications, for a fragment guess, and the like. | **Guess** panel: **Use fragments (atom groups) for generating guess** |
| **ONIOM Layer** | Define regions using different model chemistries for ONIOM calculations. | **Method** panel: **Multilayer ONIOM Model** |
| **Freeze** | Specify frozen atoms for geometry optimizations. | Adds freeze status column to the molecule specification. |
| **NMR Spin-Spin** | Specify atoms for which to perform spin-spin coupling calculations during an NMR job. | **Job Type** panel for **NMR**: **compute spin-spin couplings** |
| **Select Normal Modes** | Specify atoms with which to select normal modes in frequency calculations. | **Job Type** panel for **Frequency** or **Opt+Freq**: **Select Normal Modes** |

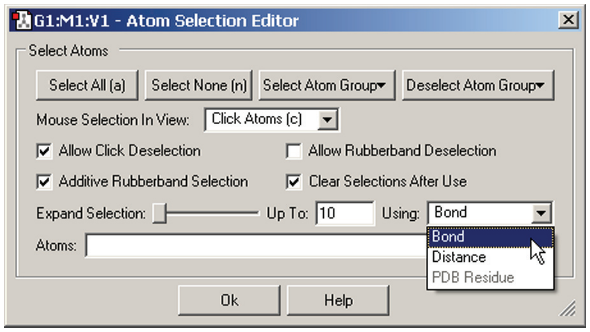
The **Class Actions** menu allows you to create a new type of atom group, to reset the atom group assignments to the default (all in the first group), to remove an atom group class and to rename a class.

There are two other important controls in this dialog:

- The **Exclusive** checkbox causes each atom to belong to exactly one atom group. When checked, if an atom is placed into an atom group, it is removed from its present group automatically. It is required for all of the atom group types used for various Gaussian calculation types. It is off by default for the Gaussian Fragment class, but the setting sticks once you enable it.
- The **Persistent Visuals** checkbox controls whether the highlighting and show/hide display settings are retained in the View window when the **Atom Group Editor** is closed. It is unchecked by default.

## The Atom Selection Editor

The **Atom Selection Editor**, reached via the **Edit=>Atom Selection** menu path, brings selection capabilities and tool preferences. It is illustrated in Figure 27.



Mouse Selection In View: Click Atoms (c)

☑ Allow Click Deselection

☐ Allow Rubberband Deselection

☑ Additive Rubberband Selection

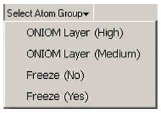
☑ Clear Selections After Use

Expand Selection: Up To: 10 Using: Bond

Atoms:

Figure 27. The Atom Selection Editor

*This dialog allows you to select all atoms, no atoms, and to select and deselect by atom group. It also sets default behaviors for click and marquee selection. You can also expand the current selection to adjacent atoms using the slider, with proximity defined by bonding, distance or PDB residue as well as a maximum value. Here, we are preparing to expand the selection to atoms bonded to already-selected atoms.*



The buttons at the top of the dialog again provide ways to select all atoms, no atoms, or the atoms within a specific atom group. The latter two buttons function as pull down menus whose contents consist of all defined atom groups for the current structure (as in the example at the left for which two different group classes are defined).

The checkboxes and popup menu in the central portion of the dialog specify defaults for the two selection modes. They have the following meanings:

| Item | Meaning |
|---|---|
| **Mouse Selection in View** | Specifies the default selection mode in View windows. |
| **Allow Click Deselection** | When unchecked, clicking again on a selected atom has no effect. |
| **Additive Rubberband Selection** | When unchecked, each marquee selection replaces the current selection rather than adding to it. |
| **Allow Rubberband Deselection** | When checked, marquee selections toggles the select status of all atoms in the enclosed region. |
| **Clear Selections After Use** | When unchecked, selections are retained even after an operation has acted on the component atoms. |

The **Expand Selection** slider allows you to expand a selection to include atoms adjacent to already-selected ones. The **Using** popup specifies how "adjacent:" atoms are identified: by bonding, by absolute distance regardless of bonding, by PDB residue. The choice made here affect what atoms will be added to the selection as the slider is moved to the right, and the **Up To** field indicates the maximum value corresponding to the right end of the slider: number of bonds, distance in Angstroms, number of residues. Thus, moving the slider all the way to the right when **Up To** is 5 and **Bond** is selected will select all atoms within 5 bonds of all currently selected atoms. When **PDB Residue** is selected, then each step selects an entire PDB residue.

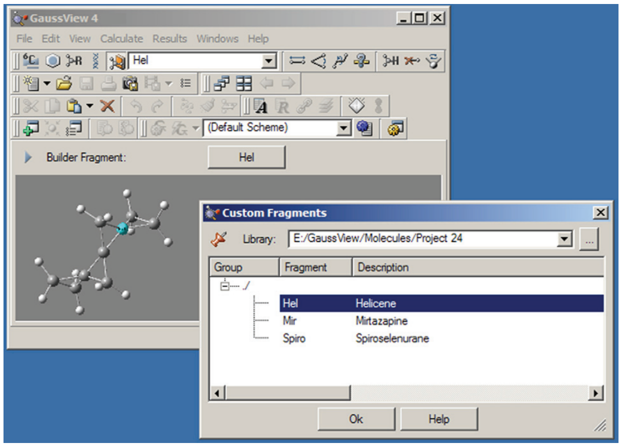
The list of selected atoms appears in the final **Atoms** field, which you can also edit directly.

## Advanced Building Features

In this section, we look at the special purpose building features designed for specific tasks and circumstances.

### Using a Custom Fragment Library

The **Custom Fragment** button can be used to access and modify a local fragment library. Clicking on it when it is inactive activates the last used custom fragment library; the first fragment within it becomes the current fragment, appearing in the area below the toolbars and in the popup menu to the right of the various building buttons. Clicking on the same button when it is selected opens the **Custom Fragments** palette, bringing up the window in Figure 28.



Builder Fragment: Hel

Library: E:/GaussView/Molecules/Project 24

| Group | Fragment | Description |
|---|---|---|
| ./ | | |
| | Hel | Helicene |
| | Mir | Mirtazapine |
| | Spiro | Spiroselenurane |

Figure 28. The Custom Fragments Window

*This palette allows you to select from the available fragments in the open library. The selected fragment will become the current fragment once the dialog is exited.*

The **Library** field at the top of the palette indicates the fragment library that is in use. Previously opened libraries are also present in the list. Additional library locations may be opened by clicking on the button labeled "**...**".

Fragment libraries are simply folders on disk, and individual fragments within a library are stored as files within that folder. Thus, creating a new fragment library consists of creating a folder at the desired location and then selecting it in this palette. The library will obviously be initially empty. Any non-fragment files within the folder are ignored, although best practice is to limit fragment library folder use solely to fragment files.

Fragments within a fragment library are organized into a series of user-defined groups. If this feature has not been used, then all fragments will be within the "root" group: i.e., / as in the figure.

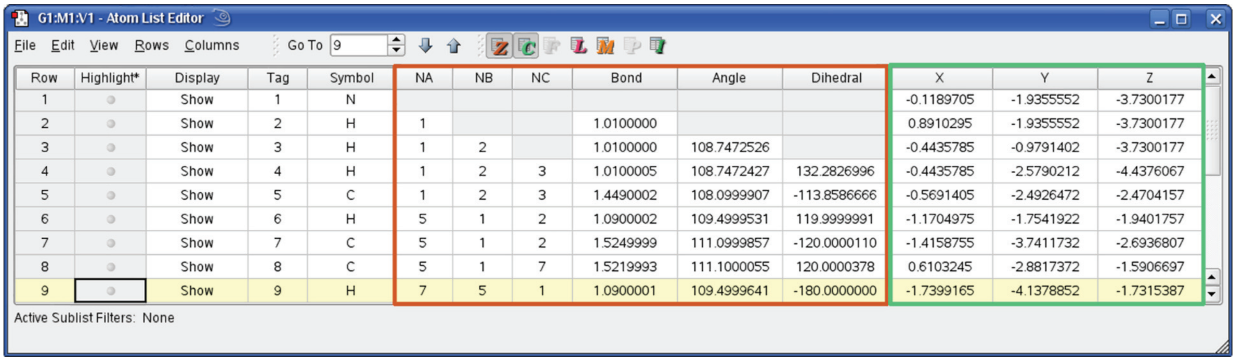
A context menu, reached by right clicking within the white fragment list area in the center of the palette, is used to manage and modify fragment libraries. It has the following selections:

- **New Group**: Create a new group within the current library. The group is initially given a generic name which you can modify. Control-G is equivalent to this menu selection (Command-N under Mac OS X).
- **New Fragment From Active Molecule**: Add the current molecule within the currently selected group within the current fragment library. A generic label and description will be set which you should edit as appropriate. In this context, Control-N/Command-N has the same function as this menu item.
- **Edit Cell**: Edit the text within the current item (group name, fragment name, fragment description). Note that the top level group name cannot be modified.
- **Delete**: Delete the currently selected fragment or fragment group. Note that the top-level fragment group cannot be deleted. The Delete key is equivalent to this menu item.

Note that fragments within a library can be updated only by removing and then readding them (there is no way to modify an existing fragment).

## The Atom List Editor

The **Atom List Editor** window is displayed when you select the **Edit=>Atom List** menu item or click on the **Atom List** button. This tool presents the coordinates and other parameters for the molecule in the active View window in an editable spreadsheet format. The window's default configuration is illustrated in Figure 29.



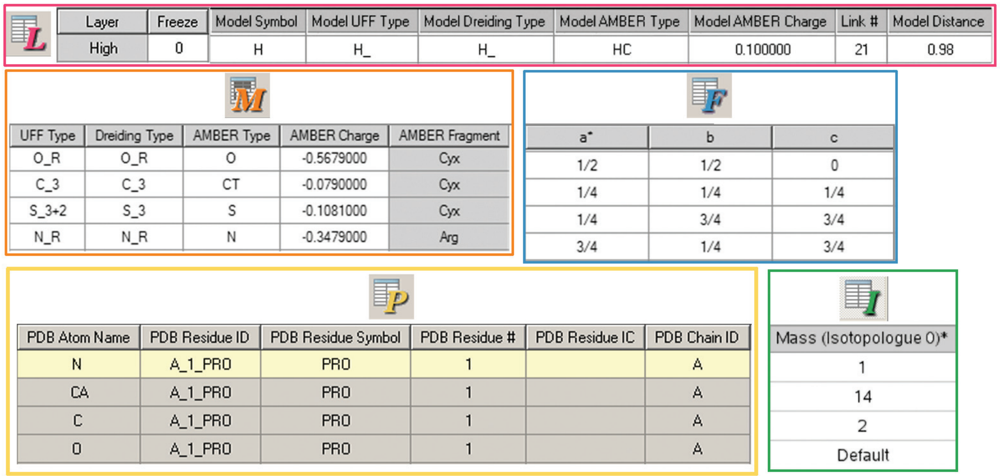
| Row | Highlight* | Display | Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral | X | Y | Z |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | ○ | Show | 1 | N | | | | | | | -0.1189705 | -1.9355552 | -3.7300177 |
| 2 | ○ | Show | 2 | H | 1 | | | 1.0100000 | | | 0.8910295 | -1.9355552 | -3.7300177 |
| 3 | ○ | Show | 3 | H | 1 | 2 | | 1.0100000 | 108.7472526 | | -0.4435785 | -0.9791402 | -3.7300177 |
| 4 | ○ | Show | 4 | H | 1 | 2 | 3 | 1.0100005 | 108.7472427 | 132.2826996 | -0.4435785 | -2.5790212 | -4.4376067 |
| 5 | ○ | Show | 5 | C | 1 | 2 | 3 | 1.4490002 | 108.0999907 | -113.8586666 | -0.5691405 | -2.4926472 | -2.4704157 |
| 6 | ○ | Show | 6 | H | 5 | 1 | 2 | 1.0900002 | 109.4999531 | 119.9999991 | -1.1704975 | -1.7541922 | -1.9401757 |
| 7 | ○ | Show | 7 | C | 5 | 1 | 2 | 1.5249999 | 111.0999857 | -120.0000110 | -1.4158755 | -3.7411732 | -2.6936807 |
| 8 | ○ | Show | 8 | C | 5 | 1 | 7 | 1.5219993 | 111.1000055 | 120.0000378 | 0.6103245 | -2.8817372 | -1.5906697 |
| 9 | ○ | Show | 9 | H | 7 | 5 | 1 | 1.0900001 | 109.4999641 | -180.0000000 | -1.7399165 | -4.1378852 | -1.7315387 |

Active Sublist Filters: None

**Figure 29.** The Atom List Editor

*The columns that are present in the table are controlled by the buttons in the toolbar. Columns corresponding to highlighted buttons are visible. Only buttons relevant to the current molecular structure are active. Individual columns may be displayed/hidden using the items on the Columns menu. You can also go directly to a specific atom (by number) using the Go To control in the toolbar.*

The default configuration of this window displays the molecule's Z-matrix and Cartesian coordinates. Different data can be selected for display using the toolbar buttons. From the left, they control Z-matrix coordinates (**Z**), Cartesian coordinates (**C**), fractional coordinates for PBC jobs (**F**), ONIOM layer assignments and related settings (**L**), Molecular Mechanics atoms types and other data (**M**), Isotope specification (**I**), and PDB file residue and chain data (**P**). Columns corresponding to the final button are read-only. Figure 26 illustrates the columns that may be present in this window. Clicking one of the lettered display icons will show or hide all columns in that group. You can also control the display of every individual column by selecting or deselecting it in the **Columns** menu.



| Layer | Freeze | Model Symbol | Model UFF Type | Model Dreiding Type | Model AMBER Type | Model AMBER Charge | Link # | Model Distance |
|---|---|---|---|---|---|---|---|---|
| High | 0 | H | H_ | H_ | HC | 0.100000 | 21 | 0.98 |

| UFF Type | Dreiding Type | AMBER Type | AMBER Charge | AMBER Fragment |
|---|---|---|---|---|
| O_R | O_R | O | -0.5679000 | Cyx |
| C_3 | C_3 | CT | -0.0790000 | Cyx |
| S_3+2 | S_3 | S | -0.1081000 | Cyx |
| N_R | N_R | N | -0.3479000 | Arg |

| a* | b | c |
|---|---|---|
| 1/2 | 1/2 | 0 |
| 1/4 | 1/4 | 1/4 |
| 1/4 | 3/4 | 3/4 |
| 3/4 | 1/4 | 3/4 |

| PDB Atom Name | PDB Residue ID | PDB Residue Symbol | PDB Residue # | PDB Residue IC | PDB Chain ID |
|---|---|---|---|---|---|
| N | A_1_PRO | PRO | 1 |  | A |
| CA | A_1_PRO | PRO | 1 |  | A |
| C | A_1_PRO | PRO | 1 |  | A |
| O | A_1_PRO | PRO | 1 |  | A |

| Mass (Isotopologue 0)* |
|---|
| 1 |
| 14 |
| 2 |
| Default |

Figure 30. Additional Atom List Editor Columns

*Beginning at the top and moving down and from left to right, these columns are controlled by the ONIOM Layers button, the Molecular Mechanics Parameters button, the Fractional Coordinates button, the PDB Info button, and the Isotope Masses button. Note that shaded columns are read-only.*

Any of the molecular parameters can be edited in this spreadsheet-like window. Atoms may be selected by clicking on their **Row** cell in the leftmost column (and deselected by clicking it a second time). The dot in the **Highlight** column causes the corresponding atoms to also be selected/deselected in the molecule's View window.

You can add additional atoms by scrolling to the bottom of the window, selecting an element in the **Symbol** column, and then clicking the **Add** button. This inserts a new row into the list (filled with default values, as in Figure 30 above).

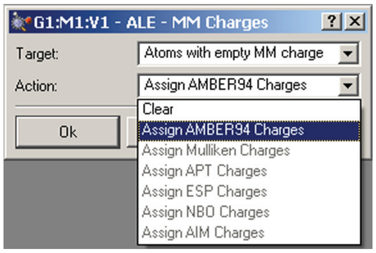
The various menu items in the **Atom List Editor** window are described below. The **File** menu includes items related to saving and printing the data in the table:

- **Export Data**: Save the data as a tab-separated format text file.
- **Print**: Print the atom list table.
- **Close**: Close the **Atom List Editor** dialog.

The **Edit** menu items allow you to modify the contents of the molecule specification:

- **Undo**: Undo the previous action.
- **Redo**: Restore the previous "undone" operation.
- **Copy Data**: Copy the data from the current row to the clipboard.
- **Delete**: Delete atoms based on the selected submenu item: **Selected Atoms** (all selected atoms), **Selected Hydrogen Atoms** (all hydrogens which are selected), **Selected Redundant Atoms** (duplicate rows within the selection), **All Atoms** (delete all atoms), **All Hydrogen Atoms** (delete all hydrogen atoms), **All Redundant Atoms** (removes all duplicate rows within the molecule specification).
- **Reorder**: Modify the display order of the table according to the item selected from the submenu:
  - **Selected Atoms by Bonding**: Order selected atoms so that bonded atoms are consecutive.
  - **Selected Atoms by Rows**: Order selected atoms by atom number (i.e., **Tag** column).
  - **Selected Atoms: Hydrogens Last**: Place hydrogen atoms last within their respective bonding group for selected atoms.
  - **All Atoms (Except the First) by Bonding**: Order atoms so that bonded atoms are consecutive.
  - **All Atoms by Row**: Order entire table by atom number (i.e., **Tag** column).
  - **All Atoms: Hydrogens Last**: Place all hydrogen atoms last within their respective bonding group.
  - **All Atoms by PDB Residue**: Order entire table by residue assignment as specified in the PDB file.
- **Z-Matrix**: Contains items useful for working with Z-matrix molecule specifications:

  - **Standardize**: Modify the Z-matrix into a form conforming to typical usage.
  - **Reconnect Selected Atoms by Bonding**: Regenerate Z-matrix entries for selected atoms by analyzing bonding.
  - **Reconnect Selected Atoms with a Nearly Invalid Dihedral**: Regenerate Z-matrix entries for selected atoms where the dihedral angle is nearly invalid by analyzing bonding (rarely needed for Gaussian jobs).
  - **Reconnect All Atoms by Bonding**: Regenerate Z-matrix entries for all atoms by analyzing bonding.
  - **Reconnect All Atoms with a Nearly Invalid Dihedral**: Regenerate Z-matrix entries for all atoms where the dihedral angle is nearly invalid by analyzing bonding (rarely needed for Gaussian jobs).
- **PBC=>Delete All Atoms Outside Cell**: Remove atoms not inside the unit cell.
- **PBC=>Translate All Atoms Inside Cell**: Translate all atoms outisde the unit cell boundary to equivalnet positions inside the cell and then delete any redundant atoms.
- **Add Hydrogens for All Atoms**: Add hydrogen atoms to the structure (typically used with PDB files).
- **Update MM Types**: Regenerate the Molecular Mechanics atoms types for the molecule. The scope of the operation, **All Atoms** or **Selected Atoms**, is specified by the submenu selection.
- **MM Charges**: Open the **MM Charges** dialog, shown in Figure 31. which allows you to assign charges to atoms for use with Molecular Mechanics methods (typically, as part of the low accuracy layer in an ONIOM job). The **Clear** option on the **Action** menu will remove any assigned charges from the specified atoms.



Target: Atoms with empty MM charge

Action: Assign AMBER94 Charges

Figure 31. Assigning MM Charges with the Atom List Editor

*This dialog is used to automatically assign charges to atoms for use in Molecular Mechanics calculations. The Target menu specifies which atoms should be assigned charges: all atoms, all selected atoms, or all atoms currently lacking an MM charge. The Action menu specifies which charge scheme should be used. Amber94 charges are always available. The other options in the list are available when they have been previously computed for the structure in a Gaussian calculation.*

The **View** menu controls atom highlighting within view windows while the **Atom List Editor** is in use. Each item in the first section is a toggle, and check mark next to it within the menu indicates that it is enabled:

- **Exclusive Highlighting**: Only allow one row within the table to be highlighted. Clicking on the dot within the **Highlight** column deletes any current highlight.
- **Z-Matrix Connectivity Highlighting**: For each highlighted atom, also highlight the other atoms used to define its Z-matrix entry (i.e., bond, angle and dihedral specification).
- **ONIOM Link Highlighting**: Display atoms for which the highlighted atom functions as a link atom for ONIOM calculations (labeled in the View window with **[Link]**), based on the contents of the row's ONIOM layer data.

The remaining items on the **View** menu have the following effects:

- **Center Highlighted Atoms in View**: Reposition the structure in the active View window so that highlighted atoms appear in the center.
- **Select/Deselect Highlighted Atoms**: Add/remove highlighted atoms from the current selection.
- **Highlight Crowded Atoms**: Turn on highlighting for atoms that are unphysically close to one another (within 0.75 Angstroms).

The **Rows** menu controls whether some or all atoms within the molecule are visible in the table and also provides some shortcuts for selecting groups of atoms:

- **Sublist Filters**: Open the **Sublist Filters** dialog for defining atom filter expressions (described below).
- **Sort Selected**: Sort highlighted atom list rows, according to the criterion selected in the submenu: **Ascending by Highlight**, or **Descending by Highlight**. The up and down arrow buttons in the toolbar are equivalent to these submenu items.
- **Sublist**: Toggle display of atoms in and/or not in the active sublist, depending on the submenu item that is chosen (**Show Sublist Atoms** or **Show Non-Sublist Atoms**). Current selections are indicated by a check mark next to the corresponding item on the submenu.
- **Select All**: Select all atoms unconditionally.
- **Invert Selection**: Deselect all currently selected atoms and select all deselected ones.
- **Select Rows of Selected Atoms** and **Select Atoms of Selected Rows**: Cause the selected atoms in the View and the selected rows in the table to be identical. The first of these gives priority to currently selected atoms, selecting corresponding table rows and deselecting others, while the second causes the View selection to match the rows selected within the table.

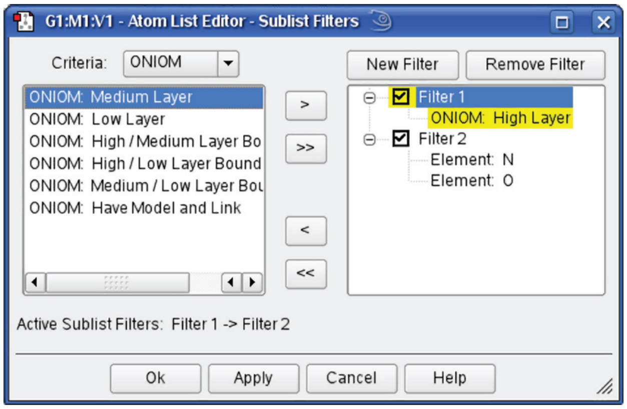
The **Columns** menu allows you to specify which columns appear in the table on an individual column basis. The first few items in the menu correspond to the default columns in the table, which are independent of the various column display buttons. The **Freeze** and **Gaussian Fragment** items further down in the list function in the same way.

You can select which columns appear for the **Z-matrix Coordinates**, **Fractional Coordinates**, **ONIOM Layers**, **PDB Info**, **Isotope Masses** and **Molecular Mechanics Parameters** buttons via the corresponding submenus. The **Cartesian Coordinates** item has the same function as the corresponding button although individual coordinates cannot be selected separately.

The **Help** menu item provides help for the **Atom List Editor**.

### Using Sublist Filters

Sublist filters are a means of limiting the visible rows within the **Atom List Editor** to a manageable number for large molecules. They are defined by means of a dialog reached with the **Atom List Editor**'s **Rows=>Sublist Filters** menu path, illustrated in Figure 32.



G1:M1:V1 - Atom List Editor - Sublist Filters

Criteria: ONIOM

Active Sublist Filters: Filter 1 -> Filter 2

Figure 32. Creating Sublist Filters

*This dialog allows you to create and apply sublist filters which are used to limit the rows which are displayed within the Atom List Editor. In this case, we apply two filters in succession: Filter 1 selects atoms in the High ONIOM layer and Filter 2 selects oxygen and nitrogen atoms within that subset.*

To use the facility, you must first create a filter using the **New Filter** button. Filters are always named **Filter n** and cannot be renamed. The filter is defined using items from within the **Criteria** list; the popup menu displays the available categories of criteria items. In the figure, we are using the **ONIOM** category to define **Filter 1**. Select one or more criteria from the list and then use the **>** button to move them to the selected filter. Although we have not done so in the example, items from different **Criteria** categories can be combined with the same filter.

The **>>** button will similarly move all items within the list. Items can be removed from filters using the **<** and **<<** items, to remove the selected item and all items (respectively). An entire filter is removed with the **Remove Filter** button.

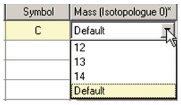
Criteria within filters are combined with an OR logic: any atom matching any criterion will be displayed (or not, according to the settings on the **Atom List Editor**’s **Rows=>Sublist** submenu). Filters are activated and deactivated by selecting/deselecting the check box to the left of their name. When only a single filter is active, all atoms matching that filter are affected. When more than one filter is active, then all active filters are applied in series, in the order in which they are listed within the dialog, according to an AND logic. For example, **Filter 2** is applied only to the matching atoms remaining after applying **Filter 1**. Subsequent filters will never enlarge the selection resulting from a previous filter, but rather only filter it further.

The available **Criteria** categories are:

- **Tags**: Select one or more atom tag numbers (serial numbers).
- **Tag List**: Select a list of atom tags.
- **Elements**: Select atoms by element type.
- **ONIOM**: Select atoms by ONIOM layer, layer boundary and/or link atom presence.
- **MM**: Select atoms having undefined Molecular Mechanics atoms types and/or MM charges.

Filters are specific to individual molecule groups, and they do not persist across different sessions for the corresponding input file. In other words, if you close and reopen the input file or if you exit and restart GaussView, current filters are lost.

### Defining Isotope Masses and Isotopologues



The **Atom List Editor** provides an easy way for specifying alternate isotope masses for atoms which are relevant for some calculation types (e.g., vibration frequency analysis). By default, Gaussian assigns the most abundant isotope to each atom in a molecular structure. You can specify a different isotope by enabling the **Isotope Masses** button. Doing so will reveal a column titled **Mass (Isotopologue 0)**. Each cell in the column contains a popup menu listing the possible isotopes for the element in that row of the table. You can select the desired isotope from the menu, or you may enter the desired value directly into the field. The **Default** choice always refers to the most abundant isotope.

You can define multiple isotopologues for the structure by adding additional columns to the table via the **Columns=>Mass=>Mass (Isotopologue n)** menu paths. These can be used for subsequent vibrational analysis visualization (discussed later).

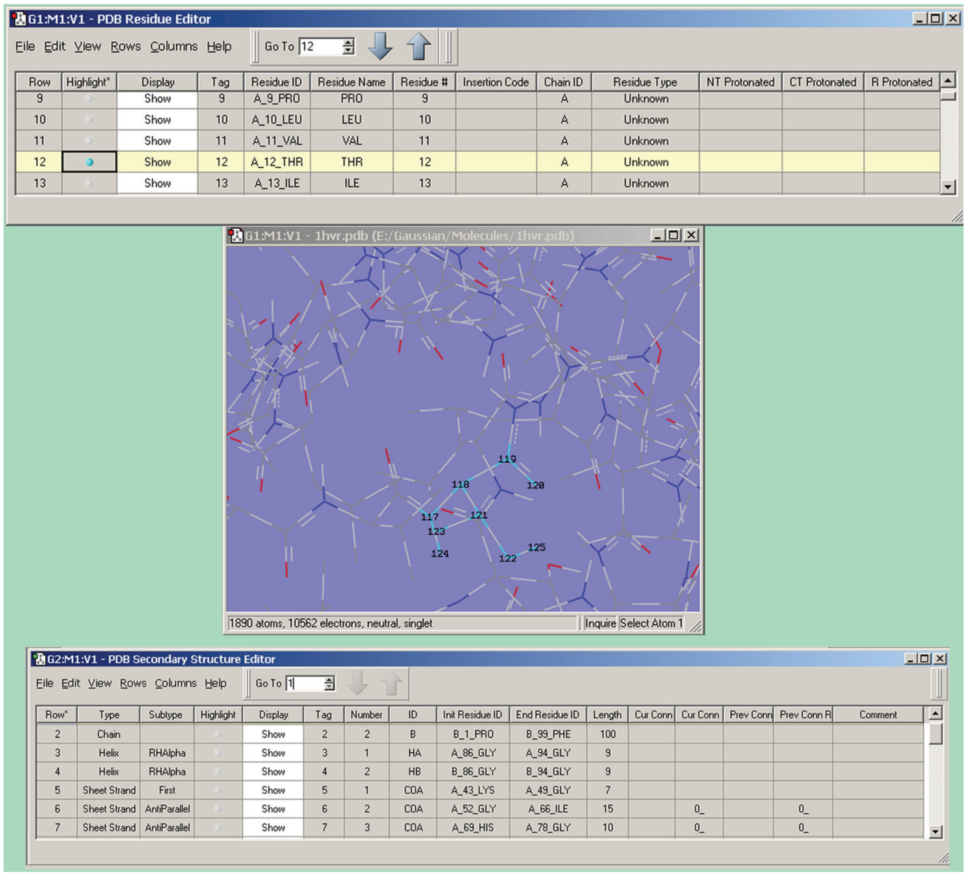
## The PDB Residue Editor and The PDB Secondary Structure Editor

Examining and modifying structures imported from PDB files may be made easier by the **PDB Residue Editor** and **PDB Secondary Structure Editor**, reached via the correspondingly named items on the **Edit** menu. They are illustrated in Figure 33.

The menus in these editors are very similar to those in the **Atom List Editor** discussed in the previous section. Briefly, they are:

- **File**: Contains items for exporting the data, printing the table and closing the editor.
- **Edit**: Contains items for undoing and redoing operations, copying data between rows, deleting all atoms or hydrogen atoms within selected residues/secondary structures, and adding hydrogens to the selected residues/secondary structures.
- **View**: Items allow you to enable/disable exclusive highlighting, center highlighted atoms in the View window, and select /deselect atoms within highlighted items.
- **Rows**: Allows you to sort the selected table rows and perform various selection operations.

- **Columns**: Used to show or hide various columns from the table.
- **Help**: Open the internal help related to the current editor.


G1:M1:V1 - PDB Residue Editor
File Edit View Rows Columns Help
Go To 12
G1:M1:V1 - 1hvr.pdb (E:/Gaussian/Molecules/1hvr.pdb)
119
118
120
117
121
123
124
125
122
Inquire
Select Atom 1
G2:M1:V1 - PDB Secondary Structure Editor
File Edit View Rows Columns Help
Go To 1

| Row | Highlight* | Display | Tag | Residue ID | Residue Name | Residue # | Insertion Code | Chain ID | Residue Type | NT Protonated | CT Protonated | R Protonated |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | ○ | Show | 9 | A_9_PRO | PRO | 9 | | A | Unknown | | | |
| 10 | ○ | Show | 10 | A_10_LEU | LEU | 10 | | A | Unknown | | | |
| 11 | ○ | Show | 11 | A_11_VAL | VAL | 11 | | A | Unknown | | | |
| 12 | ● | Show | 12 | A_12_THR | THR | 12 | | A | Unknown | | | |
| 13 | ○ | Show | 13 | A_13_ILE | ILE | 13 | | A | Unknown | | | |

1890 atoms, 10562 electrons, neutral, singlet

| Row* | Type | Subtype | Highlight | Display | Tag | Number | ID | Init Residue ID | End Residue ID | Length | Cur Conn | Cur Conn | Prev Conn | Prev Conn R | Comment |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | Chain | | ○ | Show | 2 | 2 | B | B_1_PRO | B_99_PHE | 100 | | | | | |
| 3 | Helix | RHAlpha | ○ | Show | 3 | 1 | HA | A_86_GLY | A_94_GLY | 9 | | | | | |
| 4 | Helix | RHAlpha | ○ | Show | 4 | 2 | HB | B_86_GLY | B_94_GLY | 9 | | | | | |
| 5 | Sheet Strand | First | ○ | Show | 5 | 1 | COA | A_43_LYS | A_49_GLY | 7 | | | | | |
| 6 | Sheet Strand | AntiParallel | ○ | Show | 6 | 2 | COA | A_52_GLY | A_66_ILE | 15 | | 0_ | | 0_ | |
| 7 | Sheet Strand | AntiParallel | ○ | Show | 7 | 3 | COA | A_69_HIS | A_78_GLY | 10 | | 0_ | | 0_ | |

**Figure 33.** The PDB Residue and PDB Secondary Structure Editors

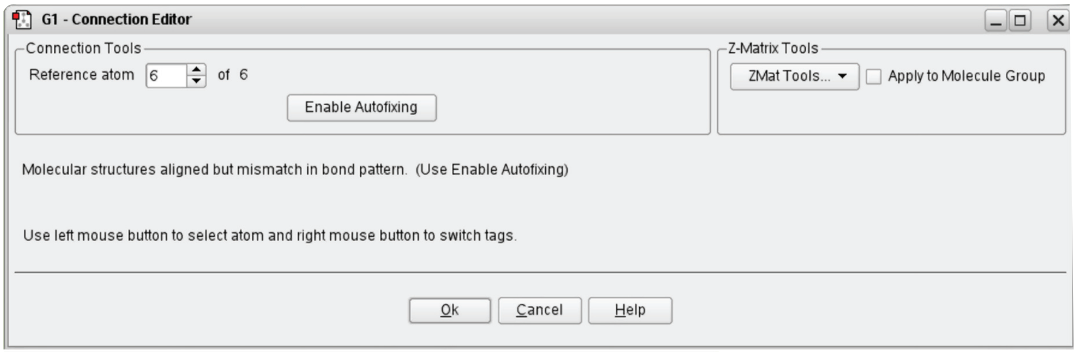
*The PDB Residue Editor (top) and PDB Secondary Structure Editor provide mainly read-only views of residue and other data assigned in PDB files. The Display column can be used to hide the atoms in certain residues/ secondary structures for easier viewing of the molecule's key features. The Highlight column can be used to highlight the atoms corresponding to the selected item. In this example, we have highlighted residue 12 in chain A making it easy to locate in the View window below.*

## The Connection Editor

The **Connection Editor**, reached via the **Edit=>Connection** menu path, can be used to determine whether proper atom ordering is maintained throughout a molecule group. You can also use it to automatically reorder atoms to align atom tags between related structures across a molecule group (useful for preparing structures for QST2 and QST3 transition structure optimizations). Manual atom reordering is also possible.

When the **Connection Editor** is active, the molecule will be analyzed to determine if the atom tags match across the entire molecule group, and the status bar will report the result. If potentially fixable mismatches are detected, the dialog will report this and suggest that the user **Enable Autofixing**. Clicking on the corresponding button will tell the **Connection Editor** to reorder the atom labels to remove these mismatches. The success or failure of autofixing will be reported on the status bar. When autofixing is active, any manual reordering of atom tags will cause autofixing to be called and remove any mismatches that might have been introduced.

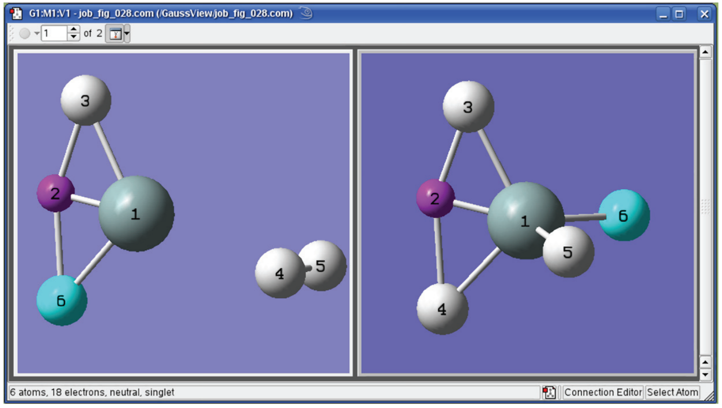
When active, autofixing can be disabled using the relabeled **Disable Autofixing** button. When autofixing is not applicable, the button is relabeled as **No Autofixing**.



Reference atom 6 of 6

Molecular structures aligned but mismatch in bond pattern. (Use Enable Autofixing)

Use left mouse button to select atom and right mouse button to switch tags.



6 atoms, 18 electrons, neutral, singlet

**Figure 34. The Connection Editor**
*The Connection Editor is used to verify and assign atom equivalences in two molecular structures. When working with a molecule group, viewing in multi-geometry mode allows easier comparison and editing. In this contrived example, we need to swap the ordering of atoms 3 and 4 in one of the models in order for the atoms to correspond properly. This can be done by clicking on the Enable Autofixing button or via a manual process.*

Atoms can also be manually reordered by using the mouse. These operations use a reference atom as their basis (see the first bullet):

- Left clicking: Designate the atom as the reference atom. This can also be done using the **Reference Atom** control.
- Middle clicking: Assign the tag one greater than the reference's item to the selected atom.
- Right clicking: Swap tags with the atom and the reference atom. The atom then becomes the new reference atom.

The **Apply to Molecule Group** checkbox determines whether the **Connection Editor**'s actions apply only to the current model or to all models within the molecule group.

The **ZMat Tools** popup allows you to perform some Z-matrix operations on the molecule or molecule group:

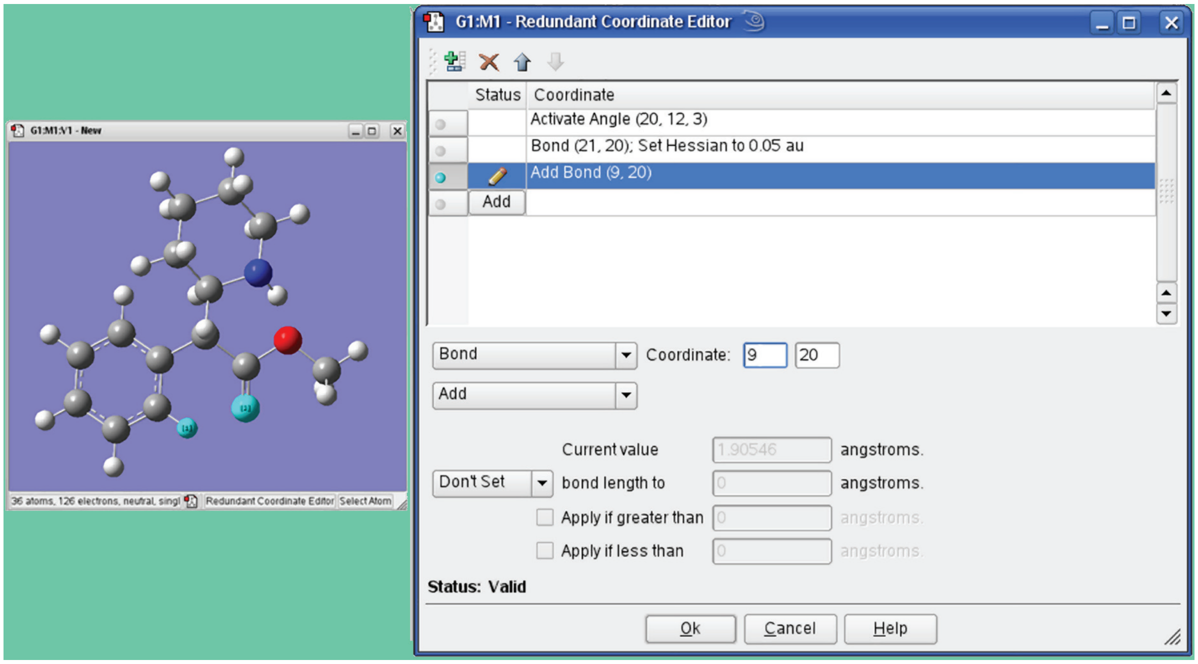
- **Sort H**: Move hydrogen atoms to the end of the atom ordering.
- **Reorder**: Reapply standard Z-matrix ordering.
- **Reconnect**: Regenerate connectivity data.

The other items on this popup menu do not apply to Gaussian.

## The Redundant Coordinate Editor

The **Redundant Coordinate Editor** allows you to create and edit redundant coordinates for use with Gaussian optimizations or potential energy surface scans. It is accessed via the **Edit=>Redundant Coordinates** menu path or the **Redundant Coordinate Editor** button. It is illustrated in Figure 35.

The central feature of this dialog is a scrollable list containing information on each of the coordinates. A pencil icon in the status column marks that coordinate as the currently active coordinate. A warning sign in the status column indicates that that coordinate is incomplete or invalid. When the currently active coordinate is invalid or incomplete, the status bar at the bottom describes the nature of the warning. The coordinate column contains a brief description of the coordinate and its parameters.


G1:M1:V1 - New
36 atoms, 126 electrons, neutral, singl
Redundant Coordinate Editor
Select Atom
G1:M1 - Redundant Coordinate Editor
Ok
Cancel
Help

| Status | Coordinate |
|---|---|
| ○ | Activate Angle (20, 12, 3) |
| ○ | Bond (21, 20); Set Hessian to 0.05 au |
| ● | Add Bond (9, 20) |
| ○ Add | |

Bond Coordinate: 9 20

Add

Current value 1.90546 angstroms.

Don't Set bond length to 0 angstroms.

☐ Apply if greater than 0 angstroms.

☐ Apply if less than 0 angstroms.

Status: Valid

Figure 35. The Redundant Coordinate Editor

*We are adding the bond coordinates for the two selected atoms so that its distance will be reported in the optimization output (even though the atoms are not in fact bonded to one another). The list in the window also shows 2 other coordinates we added.*

A toolbar at the top provides buttons for adding a new coordinate, deleting a coordinate, and moving an item up or down in the list. Adding a new coordinate creates an unidentified coordinate, which is placed in the list just after the currently active coordinate and becomes the active coordinate.

All of the available redundant internal coordinate types are supported by the various selections in the two popups in the **Coordinate** area, and the items on these menus are self-explanatory. Any additional fields required by a specific coordinate type will appear in the panel when the type is selected. See the discussion of **Opt=ModRedundant** in the *Gaussian 09 User's Reference* for more information. The **Set**/**Don't Set** popup and related fields allow you to specify the value of a coordinate or an increment to its current value.

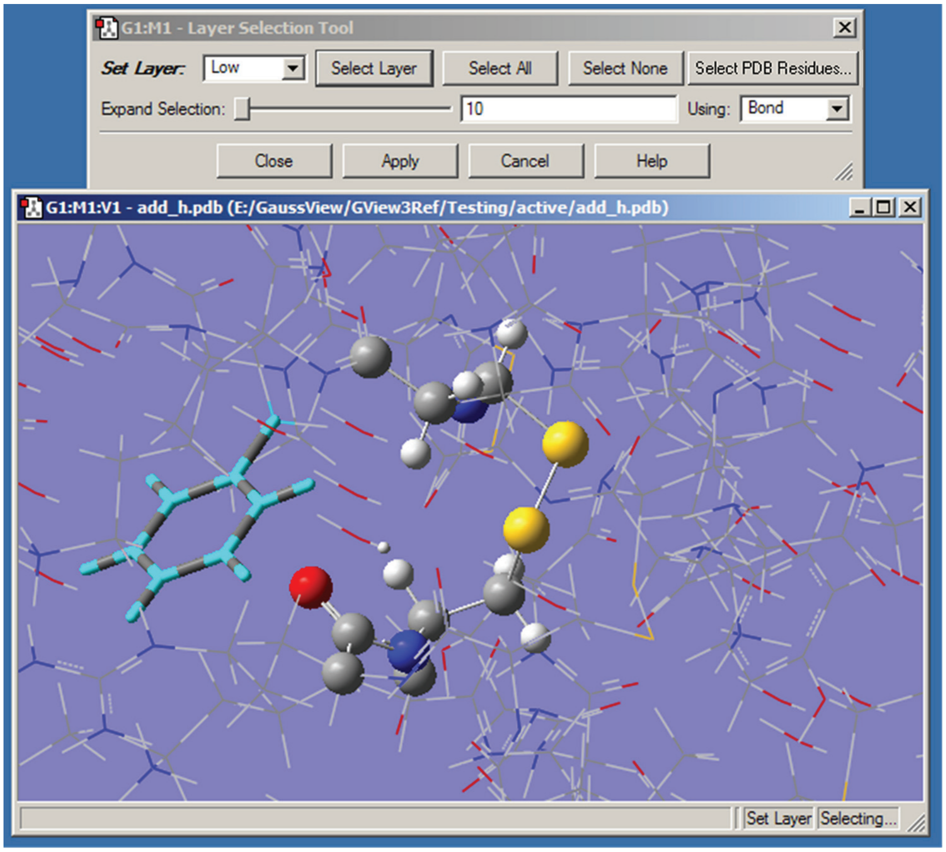
When exiting the **Redundant Coordinate Editor**, if any coordinates are still invalid or incomplete, you will be notified and given the option of continuing to edit. If you exit anyway, any invalid coordinates will be deleted.

## Specifying ONIOM Layers

Choosing the **Edit=>Select Layer** menu item or clicking on the **Select Layer** button opens the **Layer Selection Tool**. This window is used to assign atoms to ONIOM layers graphically. It is illustrated in Figure 36.

There are several methods for selecting atoms for layer assignment:

- You can use one of the buttons at the top of the dialog. The **All** button selects all atoms in the molecule, and the None button deselects all atoms. The **Layer** button selects all atoms currently assigned to the specified layer. The **Select PDB Residues** opens another selection dialog which allows you to select atoms by residue if this information was present in the PDB file corresponding to the current model (see Figure 37 below).
- Use the left mouse button to select or deselect atoms manually, continuing until all the atoms that you want have been selected. Hold down the Shift key to add to the current selection.
- Proximity-based selection: Select an atom, and then use the **Expand Selection** slider and proceed until you have selected all the atoms you need. Moving it to the right increases the distance used when selecting atoms.


G1:M1 - Layer Selection Tool
Select Layer
Select All
Select None
Select PDB Residues...
Close
Apply
Cancel
Help
G1:M1:V1 - add_h.pdb (E:/GaussView/GView3Ref/Testing/active/add_h.pdb)
Set Layer
Selecting...

Set Layer: Low

Expand Selection: 10

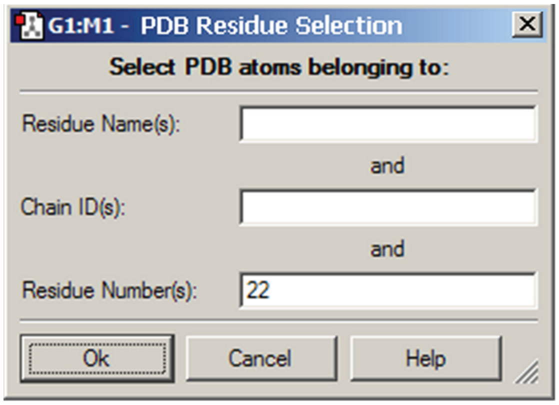
Using: Bond

**Figure 36.** Assigning Atoms to ONIOM Layers

*This dialog allows you to assign atoms to layers for ONIOM calculations. Different layers are indicated by the different display formats. Here, the atoms in the ring at the left are selected for layer assignment.*

For distance based atom selection, the distance between atoms to be selected depends on the following criteria, selected in the **Using** popup menu:

- **Bond**, which selects only atoms that are bonded.
- **Distance**, which selects an atom based solely on proximity to a current selection, regardless of whether or not it is bonded.


G1:M1 - PDB Residue Selection
Select PDB atoms belonging to:
and
and
Ok
Cancel
Help

Residue Name(s):

Chain ID(s):

Residue Number(s): 22

**Figure 37.** Selecting Atoms for Layer Assignment by PDB Residue

*This dialog allows you to specify the desired residue by residue name (type), residue number and/or chain (A or B). Omitted items act as wildcards. For example, if you enter only residue number 22, then residue 22 in both chains will be selected. Similarly, entering only a residue name will cause all residues of that type within the molecule to be selected.*

### Confirming Layer Assignments

Once atoms are selected, you must click on the **Apply** button to assign them to that layer. Note that clicking on **Apply** turns off the selection. If you close the panel without applying your changes, they will be lost.

### Layer Display Formats

By default, atoms in different layers are displayed in different formats in the View window. Using the standard settings, atoms in the High layer appear in ball-and-stick format, atoms in the Medium layer are displayed as tubes, and atoms in the Low layer are in wireframe format. These can be customized with **View=>Display Format** for the current molecule or, for all future views, via the corresponding fields in the **Molecule** panel of the **Display Format Preferences**.

## The Molecular Orbital (MO) Editor

The **Edit=>MOs** menu path and the **MO Editor** button both open the **MOs** window, illustrated in Figure 32. It is used to inspect molecular orbitals (MOs) from Gaussian calculations—MO energy and occupancy diagrams, visualized MO isovalue surfaces—as well as to quickly generate new MOs and/or visually select active-space MOs to be used for CASSCF calculations.

Resize surface window by dragging divider

Surface of selected MO

MO occupancies and energies

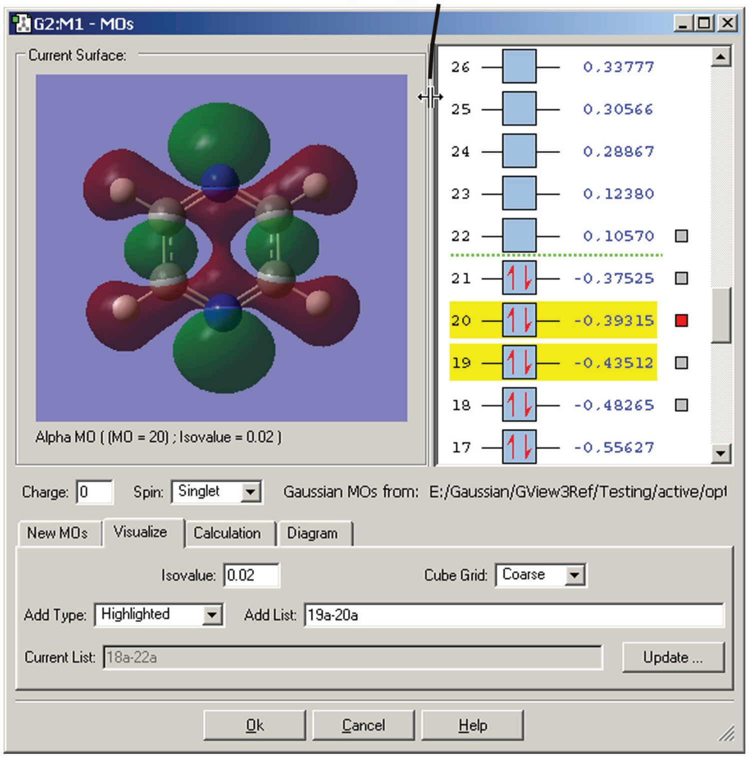
Surface boxes:
Grey = available
Red = displayed

Yellow = selected

Charge & Spin reflect and affect occupanices

Status messages

Use these panels to work with MOs



G2:M1 - MOs

Current Surface:

Alpha MO ( (MO = 20) ; Isovalue = 0.02 )

| | | | |
|---|---|---|---|
| 26 | | 0.33777 | |
| 25 | | 0.30566 | |
| 24 | | 0.28867 | |
| 23 | | 0.12380 | |
| 22 | | 0.10570 | ☐ |
| 21 | ↑↓ | -0.37525 | ☐ |
| 20 | ↑↓ | -0.39315 | ■ |
| 19 | ↑↓ | -0.43512 | ☐ |
| 18 | ↑↓ | -0.48265 | ☐ |
| 17 | ↑↓ | -0.55627 | |

Charge: 0 Spin: Singlet Gaussian MOs from: E:/Gaussian/GView3Ref/Testing/active/opt

Isovalue: 0.02 Cube Grid: Coarse

Add Type: Highlighted Add List: 19a-20a

Current List: 18a-22a

**Figure 38.** The MO Editor

*This window is used for examining molecular orbitals visually and potentially rearranging their occupancies and/or ordering for a subsequent Gaussian calculation. Here we are viewing MO 20, one of 5 available surfaces (and 2 selected MOs).*

The **MOs** dialog has its own embedded View window for displaying the molecule and surface corresponding to the currently selected MO (if available). This embedded view is read-only and cannot be used to edit the molecule. In viewing functionality, it functions almost identically to a standard View window in terms of includes keyboard and mouse controls for translating, rotating, and zooming the molecule, accessing the context menu, and so on. (See the discussion of manipulating views earlier in this chapter and that concerning surfaces in "Viewing Gaussian Results" for details.)

The size of the **Current Surface** window can be changed by resizing the entire **MOs** dialog. Its width can also be adjusted by clicking and dragging on the partition between it and the MO diagram. This adjusts the relative widths of the two windows.

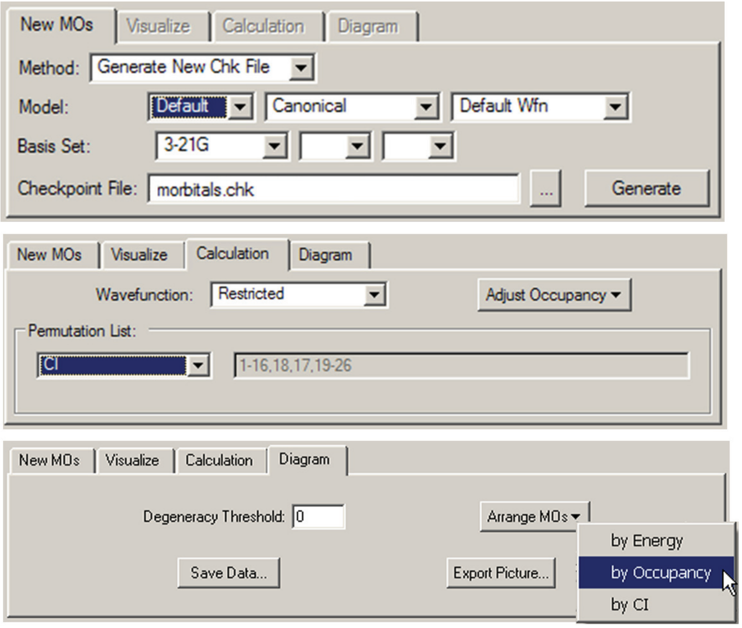
MOs can be selected for visualization, inclusion in future calculation, and other operations by left-clicking on them. Selected MOs are highlighted in yellow. If a surface is available for an MO, a small square appears to the right of the MO. The square is red for the MO whose surface is currently being viewed. Clicking on a different MO's grey square will change the **Current Surface** View to show that MO's surface.

The bottom portion of the window contains four panels:

- The **New MOs** panel is used to read-in or generate molecular orbitals.
- The **Visualize** panel allows you to generate surfaces for desired MOs.
- The **Calculation** panel allows you to modify the order of MOs for future Gaussian jobs.
- The **Diagram** panel controls the energy level and orbital occupancy display to the right of the view area.

The **Visualize** panel is visible in Figure 39. The various fields in it specify which orbitals should be visualized, along with two surface generation parameters (the isodensity value and the grid density, via the **Isovalue** and **Cube Grid** fields, respectively). The **Add Type** popup contains items which specify which MOs to visualize; its options are generally self-explanatory with the possible exception of **Current List** (regenerates the orbitals listed in the **Current List** field) and **Other** (specifies the arbitrary list of orbitals present in the editable **Add List** field). Note that GaussView attempts to keep the **Add List** and **Add Type** fields synchronized. Clicking the **Update** button will generate the requested orbital surfaces.

Figure 39 displays the other panels present in the **MO Editor** (stacked on top of one another), each of which will be discussed in the course of the remainder of this section.



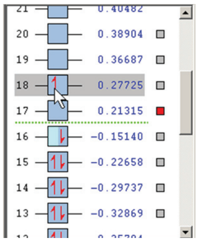
Method: Generate New Chk File
Model: Default | Canonical | Default Wfn
Basis Set: 3-21G
Checkpoint File: morbitals.chk

Wavefunction: Restricted
Permutation List: CI | 1-16,18,17,19-26

Degeneracy Threshold: 0

**Figure 39.** The MO Editor's New, Calculation and Diagram Panels
*Each panel shows a typical use for it (and not necessarily the default settings).*

### Modifying Orbital Occupancies, Molecular Charge and Spin Multiplicity



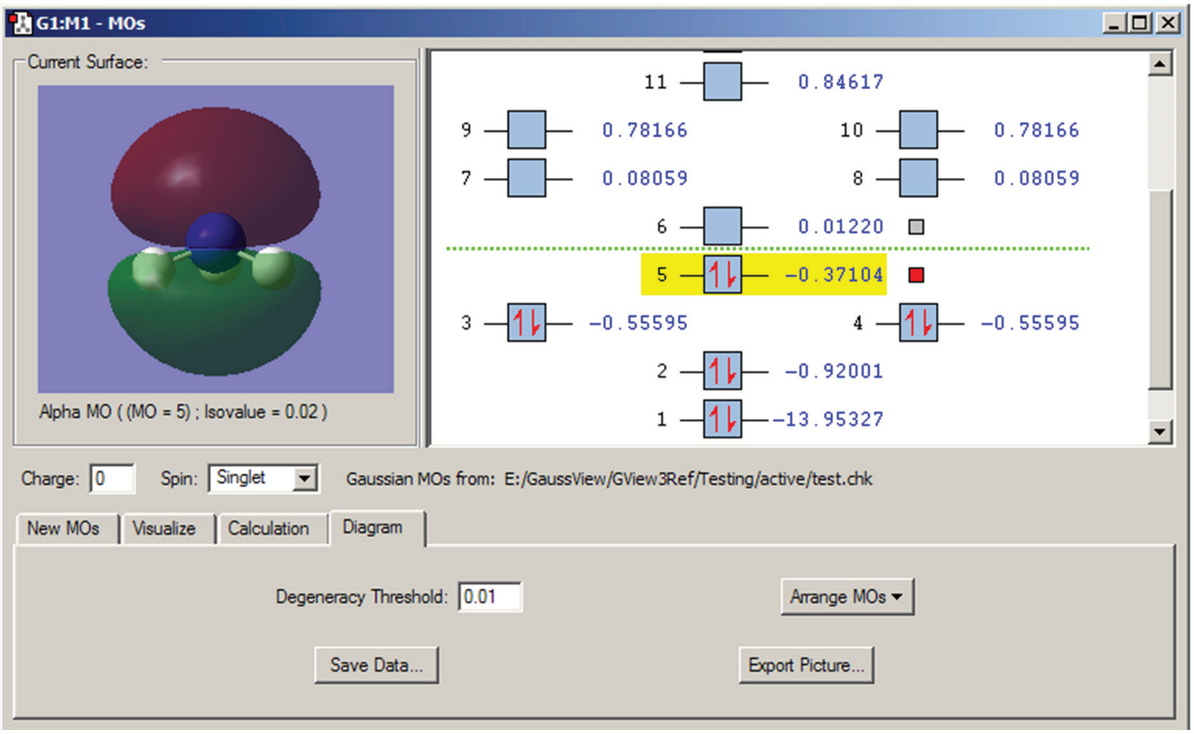
To the right of the **Current Surface** is the MO energy and occupancy diagram showing the MOs for the current molecule if available, initially arranged in order of increasing energy. Alpha and Beta electrons are represented by red up and down arrows in a blue box, respectively. Electrons can be moved from one MO to another by dragging them between the corresponding boxes. Electrons can also be added or removed from an MO by right-clicking in the MO box. Manipulating the MO occupancies in this way changes the net charge and/or spin multiplicity of the molecule as appropriate, reflected in the **Charge** and **Spin** fields. These fields can also be edited directly, and any changes will be reflected in the MO occupancies. Increasing the charge will remove electrons from the MOs, starting with the HOMO. Decreasing the charge will add electrons to the MOs, starting with the LUMO (or the HOMO if it is singly occupied). Similarly, increasing the spin multiplicity will move electrons from the highest doubly occupied MOs to the lowest virtual MOs, and decreasing the spin multiplicity will move electrons from the lowest-energy singly occupied MOs to the highest-energy singly occupied MOs. Finally, modifying the charge will also affect the spin multiplicity if the charge is changed by an odd number.

Controls in the **Calculation** panel also serve this purpose. The **Adjust Occupancies** popup contains two choices:

- **Aufbau**: Fill MOs with electrons in order of increasing orbital energy, in keeping with the current settings of **Charge**, **Spin**, and **Wavefunction**.
- **Original**: Restore the original read-in or computed orbital occupancies, modifying the **Charge**, **Spin**, and/or **Wavefunction** if appropriate.

### Controlling the Orbitals Display

The **Diagram** panel controls the orbital diagram. The **Arrange MOs** popup allows you to order orbitals by increasing energy, by occupancy, or by CI; the latter is appropriate for creating a CAS active space (see below). The **Degeneracy Threshold** sets the value below which to consider orbital energies as equal. This feature is illustrated in Figure 40.



Alpha MO ( (MO = 5) ; Isovalue = 0.02 )

Charge: 0 Spin: Singlet Gaussian MOs from: E:/GaussView/GView3Ref/Testing/active/test.chk

Degeneracy Threshold: 0.01

**Figure 40.** Degenerate Orbitals in the MO Editor

*This MO display for NH3 illustrates how degenerate orbitals appear in the orbital display area. Note that we have modified the Degeneracy Threshold from its default value of 0 to allow GaussView to detect the degenerate MOs.*

### Generating and Retrieving MOs

The **New MOs** panel allows you to read-in or generate MO data, depending on the setting of the **Method** popup. When it is set to **Load Existing Chk File**, you can read in orbital data from a checkpoint file by specifying its location and then clicking **Load**.

When **Method** is set to **Generate New Chk File**, the **Model** and **Basis Set** areas specify the calculation model for generating orbitals. The fields labeled **Model** specify the initial guess type, localization method and wavefunction type, while the desired basis set is specified in the fields below these. The fields in the second line of this panel specify the basis set to use for the Gaussian calculation. Consult the discussion of the **Guess** keyword in the *Gaussian 09 User's Reference* for more information on the various fields and choices. Clicking **Generate** will launch a Gaussian job to generate the orbital data (calculation type is **Guess=Only**).

### Rearranging Orbital Ordering

The **Permutation List** control in the **Calculation** panel displays the current orbital reordering at any given moment; it is initially empty. The popup in this area offers three choices for orbital reordering:

- **Occupancy (Alpha)**: Reorder orbitals based on the current occupancies of the alpha orbitals. This will order filled orbitals below unfilled ones, and fully occupied orbitals below partially occupied ones. Within each group, orbitals are arranged according to increasing energy.
- **Occupancy (Beta)**: Reorder orbitals based on the current beta orbital occupancies (as in the previous item). Only available for unrestricted wavefunctions.
- **CI**: Reorder orbitals so that all occupied and all unoccupied orbitals are contiguous, with each group arranged in increasing energy order. This choice is appropriate for a CAS calculation.

### Miscellaneous Options

The **Diagram** panel contains two additional controls:

- **Save Data**: Save the molecular orbital information from the MO diagram to a simple text file: orbital number, occupancy, orbital energy for each orbital and the number of frozen orbitals. For unrestricted wavefunctions, alpha and beta information will be saved in separate blocks.
- **Export Picture**: Save a graphic image of the MO diagram. You will be prompted for the filename and desired graphics format.

## Building Periodic Systems with the Crystal Editor

The **Edit=>PBC** menu path and the **Crystal Editor** button both bring up the **PBC** window. This tool is used to specify unit cells for periodic systems. In order to use this feature, as well as to perform Periodic Boundary Conditions calculations in Gaussian, you will need some understanding of periodic systems, space groups, and general related terminology. This background is assumed in this section.

The  window contains five panels:

- **Symmetry**: Specifies the dimensionality of the unit cell, the lattice system and space group constraints.
- **Cell**: Specifies dimensions of the unit cell and contains controls for repositioning & reducing cell contents.
- **View**: Specifies how many cells are displayed in each direction in the View window, as well as controlling the display/non-display of various items.
- **Contents**: Contains a list of atoms in the cell as an embedded mini Atom List Editor. Its popup also allows you to modify bonding.
- **Reduce**: Allows you to reduce the dimensionality of a unit cell (e.g., from a 3D system to a surface).

From the highest-level view, a typical process of building a periodic system might proceed as follows (consult the PBC tutorials in the GaussView online help for more detailed instructions):

[1] Use the **Symmetry** panel to specify the number of dimensions and desired space group.
[2] Add atoms to the cell using the mouse or via the Contents panel.
[3] Remove any unwanted atoms (e.g., if you used a fragment as a shortcut to creating the necessary atoms).

[4] Set the unit cell size using the **Cell** panel.
[5] Adjust bonding using the **Contents** panel if appropriate.
[6] Reduce cell contents if appropriate.
[7] Specify display properties using the View panel as desired.

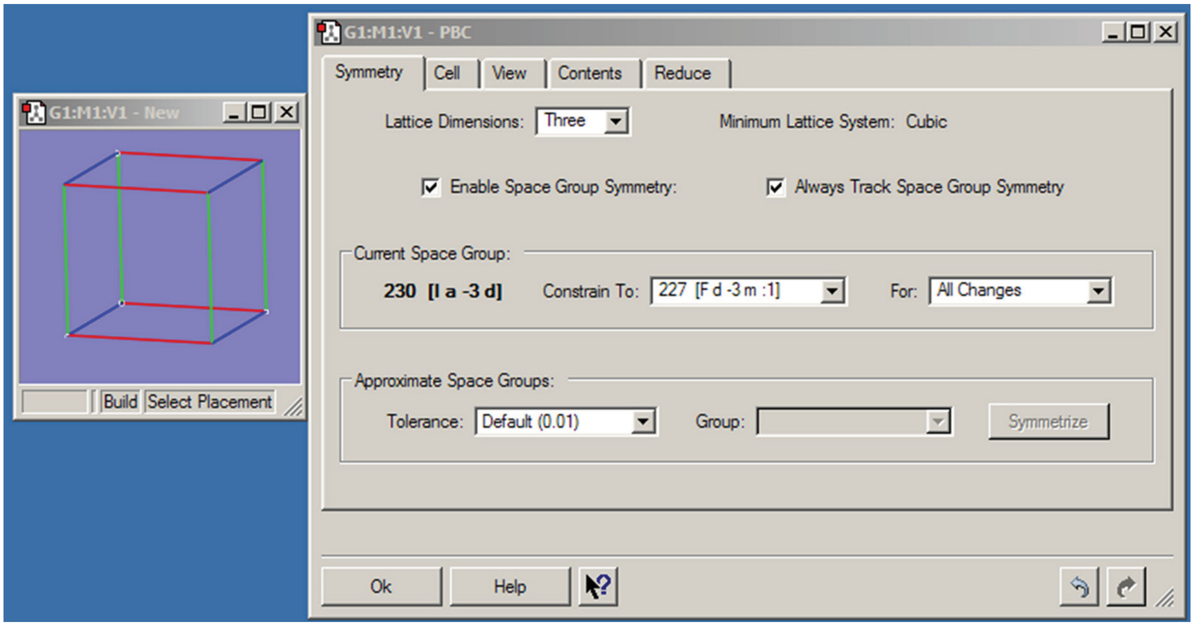
The controls in each of the PBC window panels will be described in turn in the following subsections.

### The Symmetry Panel

The **Symmetry** panel is displayed in Figure 41. It contains the following controls:

- **Lattice Dimensions**: Sets the number of dimensions in which the system has translational symmetry (i.e., is periodic): **One** for polymers, where **a** is the translation vector; **Two** for sheets, where **a** and **b** are the translation vectors, and **Three** for crystals, where **a**, **b** and **c** are the translation vectors.

  Note that the dimensionality of a lattice is not necessarily the same as the dimensionality of the corresponding cell contents. For example, the monomers of a polymer (a one-dimensional lattice) are generally not linear.
- **Minimum Lattice System**: 3D cell changes are constrained to preserve the specified lattice system. This control is read-only in the current version of GaussView (contrary to some earlier version).
- **Enable Space Group Symmetry**: Monitor space group symmetry and enforce space group symmetry constraints.
- **Always Track Space Group Symmetry**: Monitor space group symmetry during interactive changes to cell contents (e.g., continuously as the bond length slider is used) instead of only computing it after the change is completed.



Lattice Dimensions: Three
Minimum Lattice System: Cubic
☑ Enable Space Group Symmetry:
☑ Always Track Space Group Symmetry
Current Space Group:
230 [I a -3 d]
Constrain To: 227 [F d -3 m :1]
For: All Changes
Approximate Space Groups:
Tolerance: Default (0.01)
Group:

**Figure 41. The PBC Symmetry Panel**
*This panel shows settings for a 3D periodic system constrained to the indicated space group.*

These controls appear in the **Current Space Group** panel:

- **Constrain To**: Constrain changes to preserve at least the specified space group. All space groups to which the system exactly belongs are available for constraint.

- **For**: Enforce space group symmetry constraints for at least the specified type(s) of changes. **Cell Changes** refers to changes in the cell lengths or angles. **Contents Changes** refers to changes in the numbers, types and/or positions of atoms and bonds. The default is **All Changes** (i.e., both).

These controls appear in the **Approximate Space Groups** area of the panel:

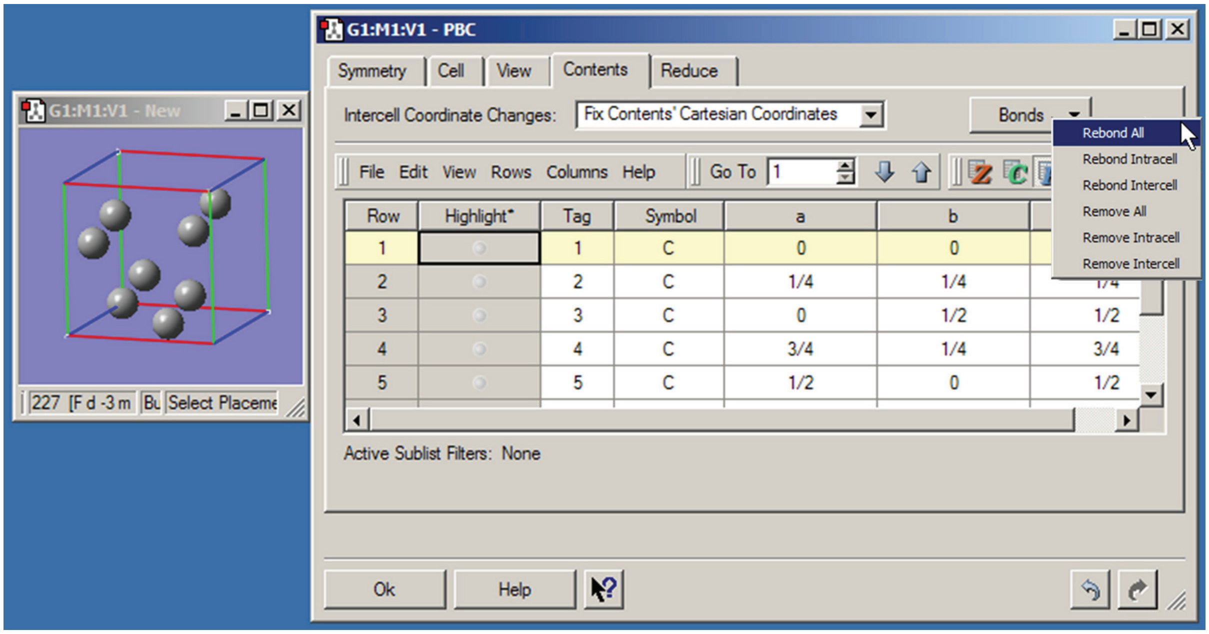
- **Tolerance**: Set the tolerance for approximately belonging to a space group, in fractional coordinates. A selection can be made from the list or you can enter any value you want into this field. Valid input consists of any floating point number (e.g., 0.25) or fraction (e.g., 1/4).
- **Group**: Set the space group to exactly symmetrize to when the **Symmetrize** button is pushed. All applicable space groups within the specified tolerance are listed.

The **Symmetrize** button will symmetrize the system to exactly belong to the specified space group.

### The Contents Panel

The **Contents** panel contains an embedded mini **Atom List Editor** which functions like the corresponding tool. It is illustrated in Figure 42. The controls at the top of the panel are:

- **Intercell Coordinate Changes**: Specify how to handle intercell coordinate changes. The selections are **Fix Contents' Cartesian Coordinates**, **Fix Contents' Fractional Coordinates**, and **Fix Cell Parameters**.
- **Bonds**: Recalculate or remove intracell and/or intercell bonds. Rebonding is based on distance criteria. The various selections on this menu are shown in Figure 42.


G1:M1:V1 - New
227 [F d -3 m
Bu
Select Placeme
G1:M1:V1 - PBC
Symmetry
Cell
View
Contents
Reduce
Bonds
Rebond All
Rebond Intracell
Rebond Intercell
Remove All
Remove Intracell
Remove Intercell
File
Edit
View
Rows
Columns
Help
Ok
Help

Intercell Coordinate Changes: Fix Contents' Cartesian Coordinates

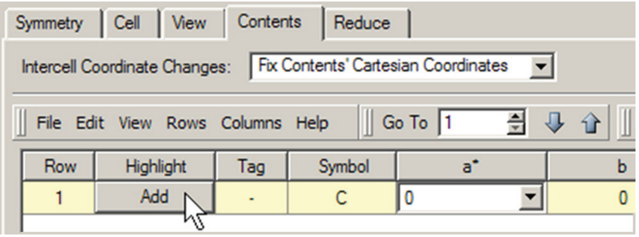
Go To 1

| Row | Highlight* | Tag | Symbol | a | b | |
|---|---|---|---|---|---|---|
| 1 | ○ | 1 | C | 0 | 0 | |
| 2 | ○ | 2 | C | 1/4 | 1/4 | 1/4 |
| 3 | ○ | 3 | C | 0 | 1/2 | 1/2 |
| 4 | ○ | 4 | C | 3/4 | 1/4 | 3/4 |
| 5 | ○ | 5 | C | 1/2 | 0 | 1/2 |

Active Sublist Filters: None

**Figure 42. The PBC Contents Panel**

*This panel displays an atom list for the contents of the unit cell. It also contains the Bonds button which allows you to rebond atoms as appropriate, typically after modify parameters with the Cell panel (see Figure 43).*


Symmetry
Cell
View
Contents
Reduce
File
Edit
View
Rows
Columns
Help

Intercell Coordinate Changes: Fix Contents' Cartesian Coordinates

Go To 1

| Row | Highlight | Tag | Symbol | a* | b |
|---|---|---|---|---|---|
| 1 | Add | - | C | 0 | 0 |

Adding atoms with this panel uses a procedure similar to that with the **Atom List Editor**. There is an **Add** button in the final row of the table (row 1 when the table is empty). In order to activate it, you must enter an element type into the column. You can also use the remaining columns to specify the fractional coordinates for the new atom. Note that additional atoms will also be added when you click **Add** in order to conform to space group constraints.

### The Cell Panel

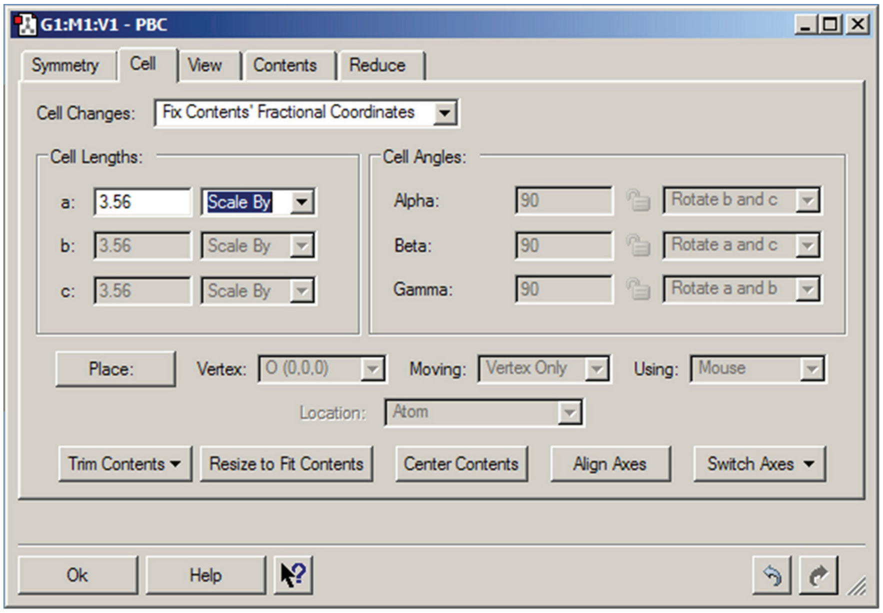
The **Cell** panel is displayed in Figure 43.

The **Cell Changes** popup specifies what should happen to the cell contents when the cell parameters are changed. When **Fix Contents' Cartesian Coordinates** is selected, the contents of the cell and their Cartesian coordinates after a change are the same as before the change, provided the atoms are still within the cell boundaries.

The setting of the **Add/Remove Atoms** checkbox affects the operation of this choice:

- If unchecked, the contents of the cell and their Cartesian coordinates after a change are the same as before the change. For example, if there is one atom in the cell with fractional coordinates (1/2, 1/2, 1/2), and the length of **a** is doubled, the contents of the cell after the change will still be one atom, but with fractional coordinates (1/4, 1/2, 1/2).
- If checked, the contents of the cell after a change is defined as whatever atoms are within the cell boundaries after the change. For example, if there is one atom in the cell with fractional coordinates (1/2, 1/2, 1/2) and the length of **a** is doubled, the contents of the cell after the change will be two atoms, with fractional coordinates (1/4, 1/2, 1/2) and (3/4, 1/2, 1/2).

When **Cell Changes** is set to **Fix Contents' Fractional Coordinates**, the contents of the cell and their fractional coordinates after a change are the same as before the change. For example, if there is one atom in the cell with fractional coordinates (1/2, 1/2, 1/2) and the length of **a** is then doubled, the contents of the cell will still be one atom with fractional coordinates (1/2, 1/2, 1/2). This option is often the more useful of the two.



Cell Changes: Fix Contents' Fractional Coordinates

a: 3.56 Scale By
b: 3.56 Scale By
c: 3.56 Scale By

Alpha: 90 Rotate b and c
Beta: 90 Rotate a and c
Gamma: 90 Rotate a and b

Vertex: O (0,0,0)
Moving: Vertex Only
Using: Mouse
Location: Atom

**Figure 43.** The PBC Cell Panel

*This panel is being used to resize the unit cell. The values in the disabled fields are predetermined by the space group to which the structure is constrained (see the Symmetry panel in Figure 35).*

The controls in the **Cell Lengths** and **Cell Angles** areas control the geometry of the cell:

- **a**, **b**, **c**: Set the length (in Angstroms) of the indicated cell vector.
- **Scale by**: Scale the length of the cell vector by a positive number.
- **Alpha**, **Beta**, **Gamma**: Set the angle (in degrees) between the other cell axes (i.e., between the **b** and **c** cell axes for the **Alpha** field). The specified angle is changed by rotating one or both of the other two cell axes, as specified in the corresponding **Rotate** field. Even for non-orthogonal cells, the rotation(s) used to change an angle are constrained to not change the other two angles.

- **Padlock icon:** If locked, freeze the specified angle at its current value. The angle is also constrained to its current value during vertex placement.
- **Rotate**: Specify the axes to rotate when the specified angle is changed. You have the choice of selecting either one or both of the other two axes.

Figure 44 illustrates the GaAs unit cell we are working on after specifying cell lengths as in Figure 43 and then rebonding in the **Contents** panel (see Figure 42).

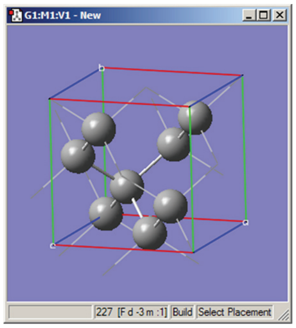


**Figure 44.** Modified and Rebonded GaAS Unit Cell

*View appearance after the operations in Figures 42 and 43.*

The fields in the next two rows of the panel control placement of the cell vertices (which define the boundaries of the unit cell):

- **Place**: Enable/disable cell vertex placement.
- **Vertex**: Specify the cell vertex to be placed.
- **Moving**: Specify whether to move the vertex only or move the whole cell.
- **Using**: Specify whether to place the vertex using mouse selection in the View window or fractional coordinates.
  - When **Using** is set to **Mouse**, the popup specifies the location type for vertex placement using mouse selection in the View window, **Atom** means that the vertex will be placed on the atom you click on, **Between Two Atoms** means that the vertex will be placed midway between the two atoms you click with the mouse, and **Any Point** means that the vertex will be placed at the point in space where you click.
  - When **Using** is set to **Coordinates**, additional fields appear for the desired fractional coordinates. Click the **Apply** button to place the vertex at the specified coordinates.

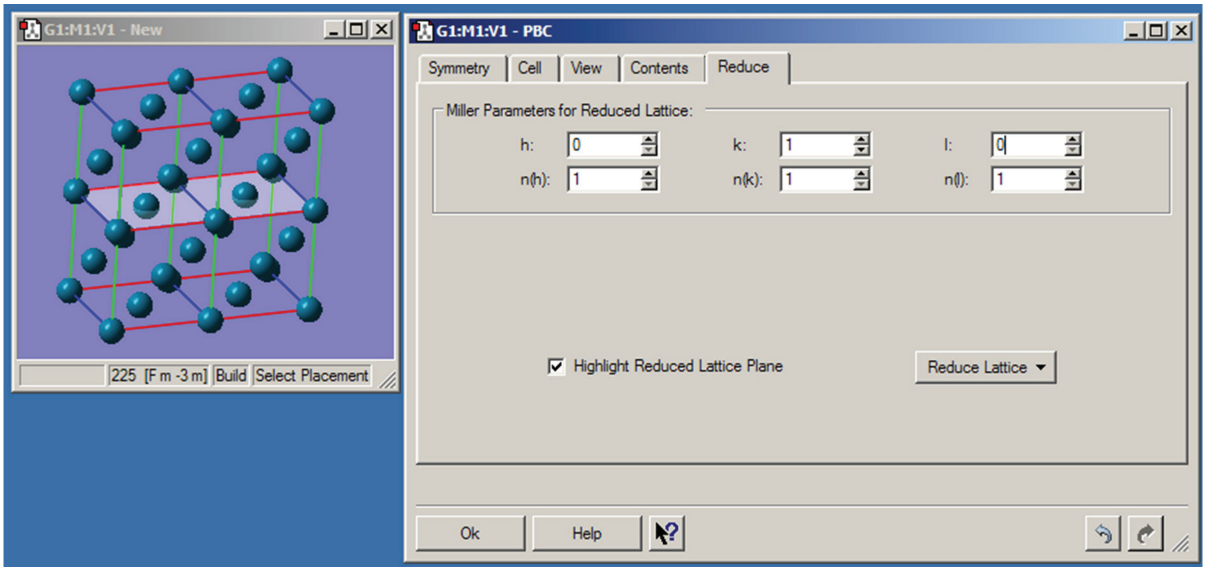
The five buttons at the bottom of the panel have the following purposes (the examples use a 3D cell):

- **Trim Contents**: Change the cell contents using the specified method. If **Delete All Atoms Outside Cell** is selected, then all atoms outside the cell boundary are deleted. If **Translate All Atoms Inside Cell** is selected, then all atoms outside the cell boundary are translated to the equivalent position inside the cell boundary. Redundant atoms are deleted. An atom is considered outside the cell boundary if one or more of its fractional coordinates is less than zero or greater than or equal to one.
- **Resize to Fit Contents**: Change the cell lengths to fit the cell contents, then center the contents. A 0.5 Angstrom cushion is added to each side of the cell.
- **Center Contents**: Translate the cell so that its center (1/2, 1/2, 1/2) coincides with the contents' center of nuclear charge.
- **Align Axes**: Align the Cartesian origin and axes with those of the cell. The cell origin (0,0,0) is first translated to the Cartesian origin. The cell is then orthogonally rotated so that the **c** cell axis is aligned with the Cartesian Z-axis. The cell is then orthogonally rotated so that the **a** cell axis is aligned with the Cartesian Y-axis. The cell is then orthogonally rotated so that the **b** cell axis is aligned with the Cartesian X-axis.
- **Switch Axes**: Switch the specified pair of cell axes. For example, if **a <–> b** is selected, then the **a** vector becomes the **b** vector and vice-versa.

## The Reduce Panel

The **Reduce** panel is displayed in Figure 45. It contains the following controls:

- **h**, **k** , **l**: Set the Miller index for the reduced lattice intercept along the **a**, **b** or **c** axis (respectively).
- **n(h)**, **n(k)**, **n(l)**: Set the multiple for the reduced lattice intercept along the **a**, **b** or **c** axis.
- **Highlight Reduced Lattice Plane**: Indicate the pending reduced lattice in the View window (see Figure 45).
- **Reduce Lattice**: Reduce the lattice by one dimension according to the specified Miller parameters.



Miller Parameters for Reduced Lattice:

h: 0
k: 1
l: 0
n(h): 1
n(k): 1
n(l): 1

☑ Highlight Reduced Lattice Plane

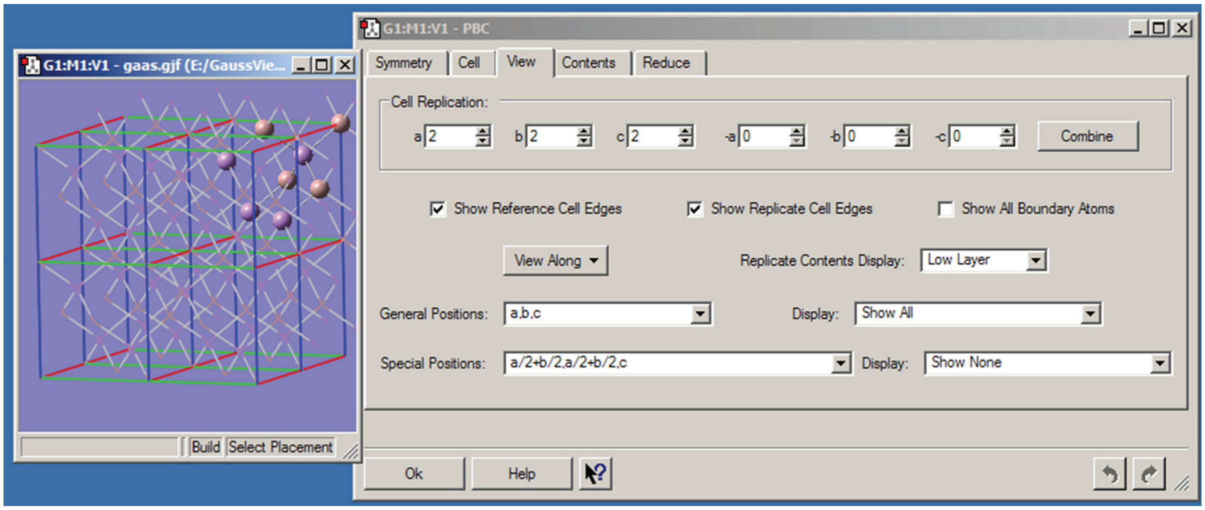
Figure 45. The PBC Reduce Panel

*This panel is used to convert a unit cell to one having a lower dimensionality. Here, we are reducing a palladium 3D cell to a surface two atoms deep. The light colored plane indicates the cut.*

## The View Panel

The **View** panel is displayed in Figure 46. It contains the following controls:

- **a**, **b**, **c**, **-a**, **-b**, **-c**: Set the number of cells to display along the specified axis (in the positive or negative direction, as indicated). This number is for display purposes only; it does not change the contents of the unit cell unless the **Combine** button is pushed. See Figure 46.
- **Combine**: Combine all of the displayed cells into one larger "supercell."
- **Show Reference Cell Edges**: Display cell edges and vertices of the reference cell.
- **Show Replicate Cell Edges**: Display cell edges and vertices of all replicate cells.
- **Show All Boundary Atoms**: Display all atoms on cell boundaries.
- **View Along**: Align the specified Cartesian or cell axis of the system with the axis perpendicular to the plane of the computer monitor.
- **Replicate Contents Display**: Specify how the atoms and bonds in replicate cells should be displayed. The choices include a normal display, a dulled-out normal display, the display format defined for one of the ONIOM layers in the **Molecule** panel of the **Display Format Preferences**, or no display.
- **General Positions**: List of equivalent positions (in fractional coordinates) for the current (constraint) space group. The **Display** popup specifies how to view the asymmetric units corresponding to the general positions for the current (constraint) space group.
- **Special Positions**: List of special positions (in fractional coordinates) for the current (constraint) space group. The **Display** popup specifies how to view the special positions for the current (constraint) space group.



Cell Replication: a 2 b 2 c 2 -a 0 -b 0 -c 0

☑ Show Reference Cell Edges ☑ Show Replicate Cell Edges ☐ Show All Boundary Atoms

Replicate Contents Display: Low Layer

General Positions: a,b,c Display: Show All

Special Positions: a/2+b/2,a/2+b/2,c Display: Show None

Figure 46. The PBC View Panel

*This panel specifies how many unit cells appear in the View window. The View window shows a 3D gallium arsenide structure. Two cells in each direction are displayed. The contents of replicate cells are displayed using the Low Layer display format (their default display mode).*

## Specifying Fragment Placement Behavior

Builder Fragment:

The small triangle above the **Current Fragment** area of the GaussView control window can be clicked to reveal some advanced options to specify how new fragments are joined to an existing molecular structure. The **Mode** popup allows you to select the settings (in which case, all fields are disabled), to specify **Custom** settings, or to restore the previously-used (**Old**) non-default settings (also nonmodifiable). You must select **Custom** in order to make changes to these items. The values for these three groups of settings can be specified in the **Building Preferences**.

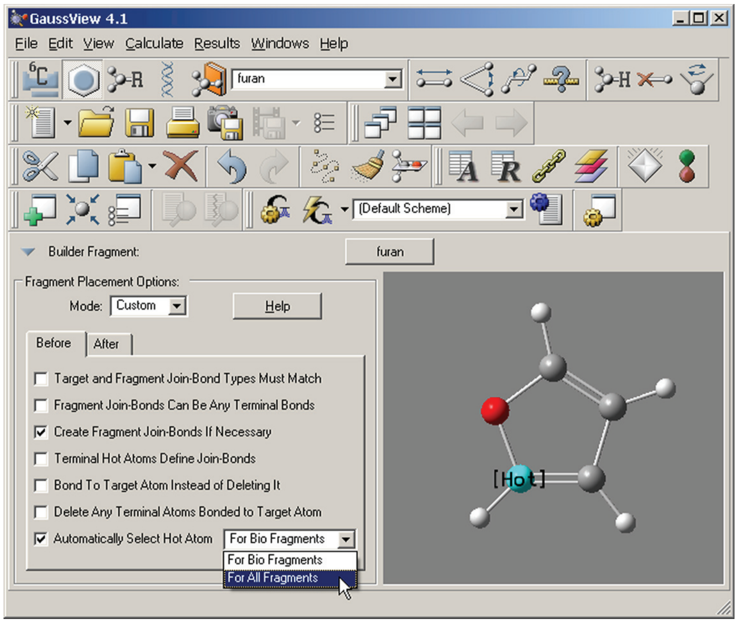
There are two panels in this area. The **Before** panel, pictured in Figure 47, sets restrictions for how fragments may be added to a structure. The **After** panel (see Figure 48) specifies how the structure is treated after a fragment is added.

Here are some preliminary definitions necessary for understanding the options in these panels:

- The *target atom* is the one selected with a mouse click.
- The *hot atom* is the atom in the new fragment that takes the place of the existing target atom when the two pieces are joined.
- A *terminal atom* is any atom bonded to only one atom.
- A *terminal valence atom* is a hydrogen atom or an open valence bonded to only one atom.
- A join-bond is a bond between the hot atom and any terminal atom. These are bonds that can be eliminated in the process of connecting the fragment to the target atom. When a fragment is joined to the target atom, there must be one join bond in the fragment for each corresponding bond to the target atom.

These are the items in the **Fragment Placement Before** panel:

- **Target and Fragment Join-Bond Types Must Match**: The selected join-bonds in the fragment must match the bond types of the target atom. Enabling this item will prevent many placements.
- **Fragment Join-Bonds Can Be Any Terminal Bonds**: Normally, only hydrogen or open valences are taken as join-bonds. When this option is on, any terminal atoms are also candidates for join-bonds. For example, the oxygen atom in formaldehyde could be used as a join-bond for ethylene because the bond type matches (double bond).



Builder Fragment: furan

Fragment Placement Options:

Mode: Custom

Help

Before | After

☐ Target and Fragment Join-Bond Types Must Match

☐ Fragment Join-Bonds Can Be Any Terminal Bonds

☑ Create Fragment Join-Bonds If Necessary

☐ Terminal Hot Atoms Define Join-Bonds

☐ Bond To Target Atom Instead of Deleting It

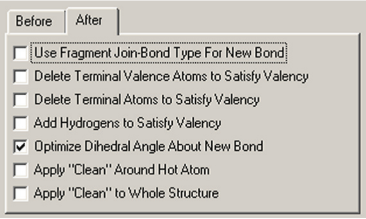
☐ Delete Any Terminal Atoms Bonded to Target Atom

☑ Automatically Select Hot Atom: For Bio Fragments (For Bio Fragments / For All Fragments)

Figure 47. Fragment Placement Restrictions

*The items in this window set restrictions on the circumstances in which fragments may be joined to an existing structure. This window shows the default values.*

- **Create Fragment Join-Bonds If Necessary**: This option will allow most fragments to be attached to any target. If the fragment does not have enough join-bonds for a given target selection, additional valences will be added to satisfy the requirement. Again, the join-bonds are deleted when fragment and target are joined as well as the target atom (on by default).
- **Terminal Hot Atoms Define Join-Bonds**: This option makes it easier to choose terminal atoms as hot atoms. Since most terminal atoms have no join-bonds, the option will use the one bond as the join-bond. However, the bond will not be deleted. This is useful when you have a central atom with more than one terminal bond, and you want to explicitly choose which terminal bond will be used to do the joining.
- **Bond to Target Atom Instead of Deleting It**. This option allows you to bond the fragment to target atom itself, deleting only the join-bonds.
- **Delete Any Terminal Atoms Bonded to Target Atom**: Remove extra terminal bonds.
- **Automatically Select Hot Atom**: This item is designed for use with biological fragments (which is its default setting). It causes GaussView to determine the hot atom dynamically. This makes it easier to build amino acid residues, etc., by producing a sensible backbone as you add residues.



Before | After

☐ Use Fragment Join-Bond Type For New Bond

☐ Delete Terminal Valence Atoms to Satisfy Valency

☐ Delete Terminal Atoms to Satisfy Valency

☐ Add Hydrogens to Satisfy Valency

☑ Optimize Dihedral Angle About New Bond

☐ Apply "Clean" Around Hot Atom

☐ Apply "Clean" to Whole Structure

Figure 48. Structure Options After a Fragment Placement

*The options in this panel allow you to select actions for GaussView to perform automatically after a fragment is added to a molecular structure. The settings in this example are the defaults.*

These are the items in the **After** panel:

- **Use Fragment Join-Bond Type For New Bond**: Normally, the bond connecting the fragment to the target bond type is determined by the original target bond. If this option is on, the fragment's bond type is used instead. This option is useful when the **Match Bond Types** option is off.

The next three items activate electron bookkeeping at the target atom site. Note, however, that non-terminal atoms are not affected. Also, GaussView does not reduce or elevate the bond type to satisfy valency requirements.

- **Delete Terminal Valence Atoms to Satisfy Valency**: Allows terminal valence atoms to be deleted to reduce overloaded valency at the target atom site.
- **Delete Terminal Atoms to Satisfy Valency**: Allows for any terminal atom to be deleted to reduce overloaded valency.
- **Add Hydrogens to Satisfy Valency**: Automatically adds hydrogen atoms to satisfy valency requirements.

The remaining options enable automatic cleaning operations, and they are self-explanatory: **Optimize Dihedral Angle About New Bond**, **Apply "Clean" Around Hot Atoms**, and **Apply "Clean" to Whole Structure**.

# Opening, Displaying and Saving Molecules and Views

## Customizing and Manipulating Molecule Views

GaussView contains a variety of controls and features for customizing the displays in View windows. These may be accessed via the **View** menu, and also via toolbar icons in some cases. The **View** menu may also be accessed by clicking the right mouse button in an open area of any View window or other molecule display.

### Centering the Molecule

The **Center** button and the **View=>Center** menu item centers and resizes the image in the active View window to make the most efficient use of the workspace.

### Viewing Optional Display Items

Several **View** menu options toggle the display of optional items within a View window:

- **View=>Hydrogens**: Display of hydrogen atoms in the View window (initially on).
- **View=>Dummies**: Display of dummy atoms if present (initially on).
- **View=>Labels**: Display numeric labels indicating atom sequence numbers (initially off).
- **View=>Symbols**: Display the chemical symbol for each atom (initially off).
- **View=>Bonds**: Display bonds between atoms (initially on).
- **View=>Synchronize**: Coordinate mouse actions in synchronized views.
- **View=>Cartesian Axes**: Display X,Y,Z axes (initially off). This feature is illustrated in Figure 49. Initially, the origin of the axes is in an arbitrary position (sometimes located on atom 1), and it remains fixed despite changes to the molecule. Use the **Edit=>Reorient** menu item to move the origin to the molecule's current center of mass.
- **View=>Stereochemistry**: Display the chirality of any chiral centers (initially off).
- **View=>Positioning Tools**: Open positioning toolbar in View window (initially off).

You can specify default values for these items via the **General** panel of the **Display Format** dialog (**View** menu) or the **Display Format** panel of the preferences. You can also exclude labels and symbols on hydrogen atoms or hydrogen and carbon atoms using the **Exclude View Labels** and **Exclude View Symbols** items in the **Text** panel of the **Display Format Preferences** (both default to excluding no atom types). Finally, the size of textual labels can be adjusted using the **Size** field in the **Text** panel of the **Display Format Preferences**.

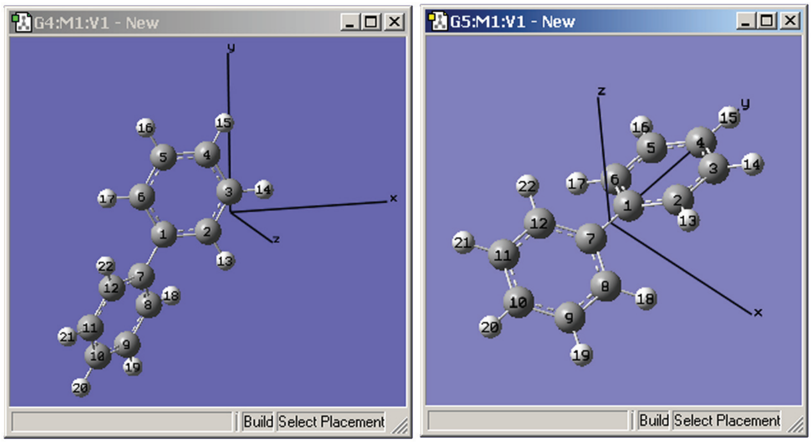


**Figure 49.** Displaying Cartesian Axes

*These windows illustrate GaussView's Cartesian Axes display option. The window on the left shows the initial position of the axes (which is quite arbitrary), and the one on the right shows the origin's new position after using the Edit=>Reorient menu item.*

## Molecule Positioning Tools

Figure 50 illustrates the molecule positioning toolbar, which is accessed with the **View=>Positioning Tools** menu item.

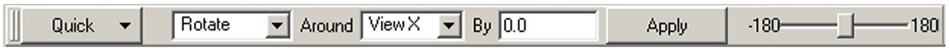


Figure 50. The Positioning Toolbar

For all of the tools, the view's X, Y and Z directions are the horizontal, vertical and depth of the window, and the molecule X, Y and Z directions are those indicated by the Cartesian axes. The various controls are described individually below (moving across the toolbar from left to right):

- The **Quick** popup contains items which center the molecule in one or more view directions or align axes on the molecule with that of the view. For example, the **Center** and **Center X** items center the molecule within the window and with respect to the window's X-axis (i.e., horizontally), while the **Mol X -> View Z** item aligns the molecule's X-axis with the View window's Z-axis. Other items work analogously.
- The second popup menu indicates whether the molecule will be rotated or translated in order to perform the repositioning when the **Apply** button is pushed. The next two fields also control the operation.
- The **Around** field specifies the axis about which the molecule will be rotated (active when the previous popup is set to **Rotate**). When **Translate** is selected in the initial field, then the label changes to **Along**.
- The **By** field specifies the amount of rotation or translation.
- The final slider provides another way to specify the amount of movement. As you adjust the slider, the molecule moves immediately in the direction and manner specified by the first two fields (and the **By** field is ignored).

## Molecule Display Formats

The **Display Format** button and the **View=>Display Format** menu item both open the **Display Format** dialog. Each panel in this dialog also has a twin within the **Display Format Preferences**. We will consider the **General**, **Text** and **Molecule** panels here and will consider the **Surface** panel later in this book.

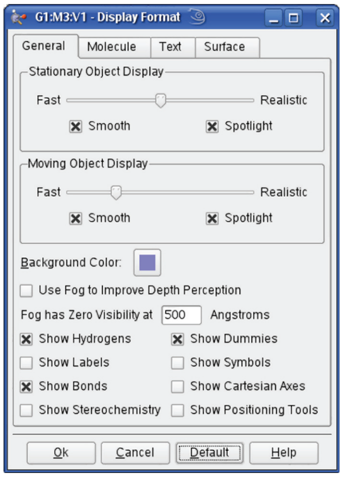
### The General Panel

The items in the **General** panel control molecule display quality, items displayed in the view (as mentioned above), and the fog feature. It is illustrated in Figure 51.

The options in the top part of this panel govern how the molecule appears both when it is being moved in the View window by mouse action and when it is not moving. On slower systems, it can be often useful to set the slider more toward the **Realistic** end of the scale for **Stationary Object Display** and more toward the **Fast** end of the scale for **Moving Object Display**.

The **Smooth** checkboxes enable/disable smoothing in the display, and the **Spotlight** checkboxes enable/disable simulated spotlighting on the window contents.

You can change the View window background color by clicking on the color chip labeled **Background Color**, and selecting a new color using the color selection dialog.



G1:M3:V1 - Display Format

General | Molecule | Text | Surface

Stationary Object Display

Fast — Realistic

☒ Smooth ☒ Spotlight

Moving Object Display

Fast — Realistic

☒ Smooth ☒ Spotlight

Background Color:

☐ Use Fog to Improve Depth Perception

Fog has Zero Visibility at 500 Angstroms

☒ Show Hydrogens ☒ Show Dummies

☐ Show Labels ☐ Show Symbols

☒ Show Bonds ☐ Show Cartesian Axes

☐ Show Stereochemistry ☐ Show Positioning Tools

**Figure 51.** Display Format General Panel

The **Use Fog to Improve Depth Perception** checkbox causes more distant atoms in the View window to recede to invisible, allowing nearer atoms to become more distinct. The **Fog has Zero Visibility at** field controls the depth at which atoms become completely invisible.

This feature is illustrated in Figure 52. In this example, the lefthand illustration shows the molecule with the fog feature disabled. In the righthand illustration, fog is turned on, and the frontmost atoms are much more distinct than more distant ones.

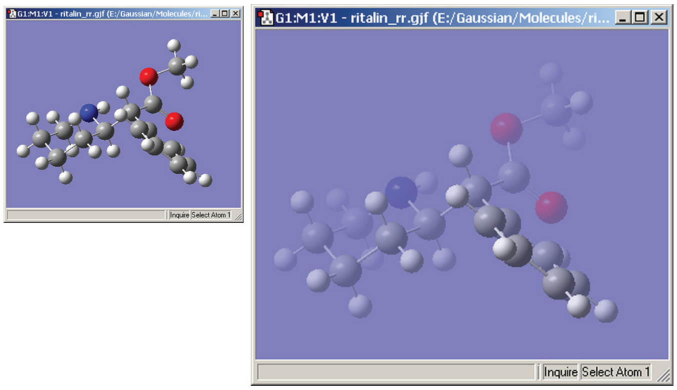
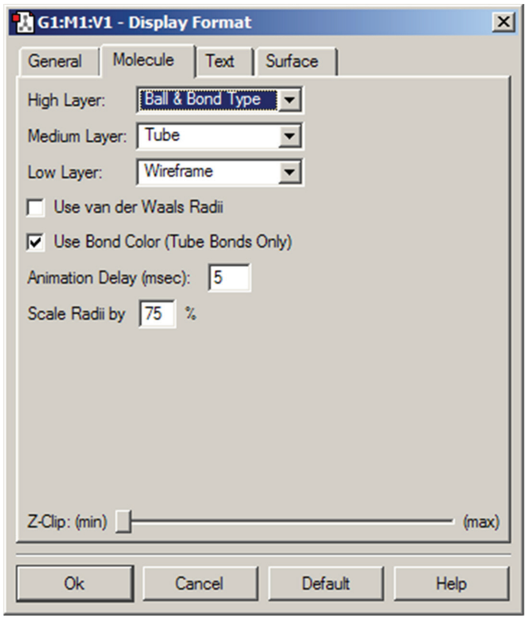

G1:M1:V1 - ritalin_rr.gjf (E:/Gaussian/Molecules/ri...
Inquire Select Atom 1
G1:M1:V1 - ritalin_rr.gjf (E:/Gaussian/Molecules/ri...
Inquire Select Atom 1

**Figure 52.** The Fog Depth Display Feature
*Compare the display types between the two windows to understand the effect of fog.*

## The Molecule Panel

The options in this panel control how atoms and bonds appear in the View window. The three popup menus specify how atoms in each of the three ONIOM layers will be displayed. If the ONIOM facility is not being used, then the setting for the **High Layer** is used. The **Molecule** panel is shown in Figure 53.

The layer display settings are also used by some other GaussView features unrelated to ONIOM (e.g., displaying atoms at the boundaries of PBC unit cells).



High Layer: Ball & Bond Type

Medium Layer: Tube

Low Layer: Wireframe

☐ Use van der Waals Radii

☑ Use Bond Color (Tube Bonds Only)

Animation Delay (msec): 5

Scale Radii by 75 %

Z-Clip: (min) (max)

**Figure 53.** The Display Format Molecule Panel

*The various items in this panel control various aspects of molecule displays.*

The various supported display types are:

- **Ball & Stick**: Molecule appears as a ball and stick model, with all types of bonds represented by single sticks. This is the default.
- **Ball & Bond Type**: Molecule appears as a ball and stick model with single bonds represented by single sticks, and multiple bonds represented by multiple sticks, or in the case of aromatic systems, by dotted lines.
- **Tube**: Molecule appears as a tube model with no indication as to bond type. Atom types are indicated by color bands on the tubes.
- **Wireframe**: Molecule appears as a series of thin lines, colored by atom type and indicating bond type via the number of lines.
- **None**: Atoms are invisible (useful only with multilayer models).

The **Use van der Waals Radii** checkbox and **Scale Radii by** field cause the atoms in the View window to be displayed at the indicated scaling of the van der Waals covalent radii. Using a scaling value of 150%-200% will produce a space filling-like molecular display, as in Figure 54.

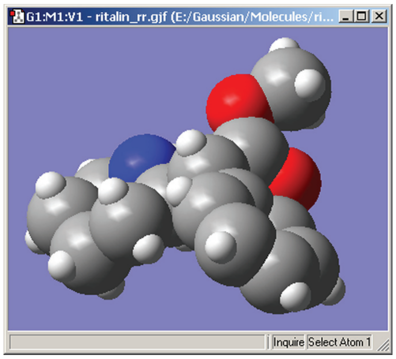


**Figure 54.** A CPK-Like Display

The **Z-Clip** slider may be used to remove the frontmost portions of the image to allow views into the interior of the molecular display.

The **Use Bond Color** checkbox controls whether bonds are partially or entirely colored by atom type in the tube display format. The two options are illustrated in Figure 55.

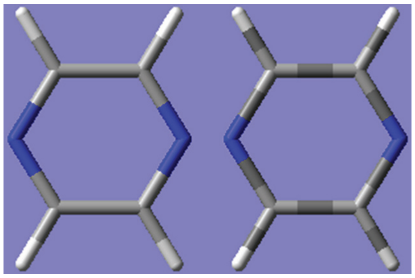
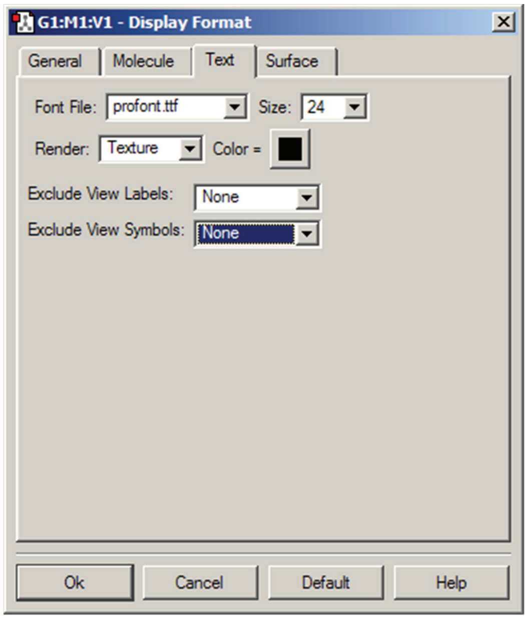


Figure 55. Tube Display Formats

*These windows show pyrazine using the tube display format without (left) and with (right) the Use Bond Color item checked. The format on the left is the default.*

### The Text Panel

The **Text** panel of the **Display Format** dialog controls the font and color of atom labels and symbols as well as allowing you to exclude certain atoms from labeling as previously mentioned. It is illustrated in Figure 56.



Font File: profont.ttf
Size: 24
Render: Texture
Color =
Exclude View Labels: None
Exclude View Symbols: None

Figure 56. The Text Panel of the Display Format Dialog

*This panel allows you to specify various aspects of text labeling of atoms.*

The **Font File** menu allows you to select from several font files provided with GaussView. The **Size** field specifies the relative type size: type resizes with the molecule as you zoom in or out. The **Render** field specifies the type rendering method, and the **Color** field specifies the type color. Note that font sizes are generally limited to those included on the **Size** menu.

## Customizing Display Colors

The **Colors Preferences** allow you to customize the coloring of View window backgrounds, atoms (elements), bonds, surfaces and vibration vector displays. The dialog is illustrated on the left in Figure 57.

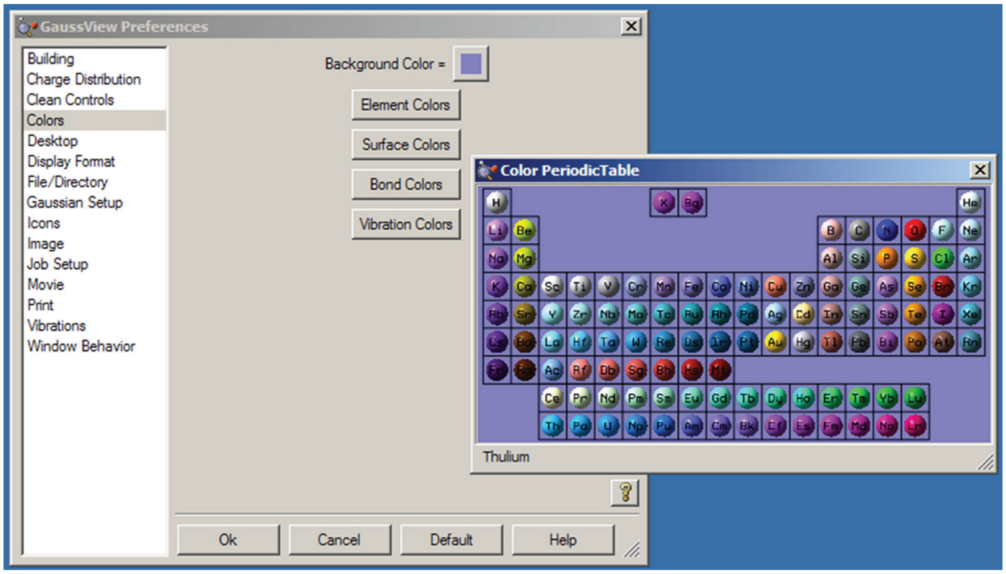

GaussView Preferences
Building
Charge Distribution
Clean Controls
Colors
Desktop
Display Format
File/Directory
Gaussian Setup
Icons
Image
Job Setup
Movie
Print
Vibrations
Window Behavior
Background Color =
Element Colors
Surface Colors
Bond Colors
Vibration Colors
Color PeriodicTable
Thulium
Ok
Cancel
Default
Help

Figure 57. Customizing GaussView Colors

*The Colors preferences dialog appears on the left, and the Element Colors preferences appears on the right.*

The items in the **Colors Preferences** dialog control the coloring of the following items:

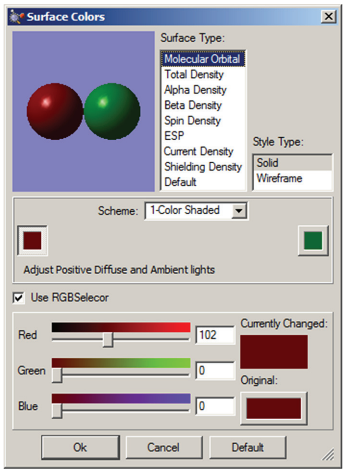
- **Background Color**: Background color in view windows. Click on the color chip to modify it.
- **Element Colors**: Element-based atom coloring. This button brings up a periodic table indicating the default color for each element (see Figure 57). Click on any element to change its default color.
- **Surface Colors**: Specifies colors for surfaces (discussed below).
- **Bond Colors**: Sets coloring for bonds in each of the various display types. The dialog is similar to the one in Figure 52, and it displays the selected color on a sphere. Don't be confused by this; the selected colors will be used to color the bonds, not the atoms.
- **Vibration Colors**: Sets the coloring of the dipole derivative and displacement vectors in vibrations displays. Again, although the color selector is similar to the one in Figure 58, the color selected will be used to color the displayed vectors, not the atoms.

### Specifying Colors

The dialog in Figure 58 is used to specify coloring for single-color surfaces. For surfaces types having positive and negative lobes (phases), two colors are specified (as in the figure, which specifies colors for MO surfaces). The dialogs for other **Colors Preferences** items are similar.

The fields at the top of this example dialog allow you to select the surface type and display style (in dialog for other items, the appropriate items are substituted for these). The most important fields are located in the center of the dialog. The Scheme popup allows you to select the type of coloring that is applied to the object. The **1-Color Shaded**, **2-Color Shaded**, **3-Color Shaded**, and **4-Color Shaded** items select gradient-filled coloring, consisting of shades of the indicated color (**1-Color Shaded**) or blends between the specified colors (2 or more colors). Keep in mind that less is more with gradients when good taste prevails. The **1-Color Flat** colors the object using the specified color in a solid mode, without creating any illusion of three-dimensional shape.

Clicking on any of the color chips in this area allows you to modify that color. Note that two-lobed surfaces will have two sets of color chip(s), placed on the left and right sides of the dialog. If the **Use RGB Selector** checkbox is selected, then you can use the sliders below it to specify the RGB values for the desired color. If it is unchecked, then the system color selection utility will be invoked.



Scheme: 1-Color Shaded

Adjust Positive Diffuse and Ambient lights

☑ Use RGBSelecor

Red 102

Green 0

Blue 0

**Figure 58.** Surface Coloring Preferences

*This dialog allows you to customize the colors used for surfaces.*

## Adding and Synchronizing Views

**View=>Add View** menu item and the **Add View** button may be used to add a new View window for the current model. This view is independently adjustable, and begins with the default settings (rather than those of the current View window).

The **View=>Synchronize** menu item can be used to link distinct views of the same model or different models with respect to mouse-based view operations: rotation, translation, zooming, etc. You must enable this item for each View window that you want to synchronize. Note that synchronization does not affect other display choices and that views are automatically synchronized with respect to structural changes.

## Selecting View Windows

The **Windows** menu contains items that control which view windows are open and/or visible. All views and associated dialogs of a molecule group can be hidden/shown by checking/unchecking the corresponding item in the **Windows=>Molecule Groups** submenu. Individual view windows can be hidden or shown using the corresponding item at the bottom of the main **Windows** menu. Selecting a window here makes it the active view. Note that hiding is not the same as closing and is solely for the purpose of managing screen space. It is also different from minimizing a window as no icon is visible for a hidden window.

The **Show All** and **Show None** items on the **Windows=>Molecule Groups** submenu display and hide windows for all model groups (respectively). The related **Windows=>Minimize All**, **Windows=>Restore**, and **Windows=>Restore All** menu items respectively minimize, open the active view, or open all minimized view windows (but not hidden ones). The **Windows=>Close** and **Windows=>Close All** items close the active window or all view windows (respectively).

The **Windows=>Previous** and **Windows=>Next** items (and the equivalent **Previous** and **Next** buttons) activate the previous or next window in sequence.

Finally, the **Windows=>Cascade** and **Windows=>Tile** menu items (and the equivalent **Cascade** and **Tile** buttons) arrange all windows in an overlapped pile or resize them and rearrange them on the screen so that the maximum number are simultaneously visible (all of them, if possible).

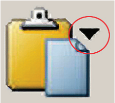
## Working with Molecules and Files

In this section, we will discuss operations related to molecules and molecule groups, including their storage in external files.

### Pasting Molecules into the View Window

The **Edit=>Cut** and **Edit=>Copy** menu items and the corresponding **Cut** and **Copy** buttons can be used to cut or copy the entire structure in the current model to the system clipboard. Note that any atom selection within the model is ignored.

The **Edit=>Delete Molecule** menu item and the **Delete Molecule** button can be used to remove the structure in the current model, discarding it without copying it anywhere.



There are several options for pasting molecules from the clipboard. The **Edit=>Paste** menu item accesses a slideoff menu containing three items. These items can also be reached via the small downward pointing triangle on the **Paste** button. Clicking on the **Paste** icon itself (avoiding the triangle's panel) selects the **Replace Molecule** item.

The items on the **Paste** submenu are:

- **Edit=>Paste=>Add to Molecule Group**: Create a new model within the current molecule group, and place the structure on the clipboard into it.
- **Edit=>Paste=>Replace Molecule**: Remove the structure in the active window and place the one on the clipboard there instead.
- **Edit=>Paste=>Append Molecule**: Add the molecule on the clipboard to the active model as a separate fragment.

### File Drag and Drop under Windows

On the Windows platform, files can be added to the current molecule group by dragging them from an Explorer window or other source and dropping them onto a View window. Dragging and dropping with the left mouse button will load the contents of each file and add it to the molecule group.

By default, file contents are placed as new molecules within the current molecule group. However, dragging and dropping multiple files with the right mouse button will open a context menu with these options:

- **Add all files to this molecule group**: The files are appended to the current molecule group (the default).
- **Append files to this molecule**: The contents of the file(s) are appended to the current molecule (rather than creating new frames within the current molecule group).
- **Separate new molecule group for each file**: A new molecule group is created for each file and the current molecule group is unchanged.
- **Single new molecule group for all files**: One new molecule group is created for all of the files, with each file comprising one molecule (frame) within it, and the current molecule group is unchanged.

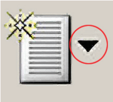
The wording of the options differs slightly when only a single file is dragged, and the final option does not appear.

### Adding a Model

The **File=>New** menu item accesses a slideoff menu containing two items. The items on the **New** submenu are:

- **Create Molecule Group**: Create a new View window corresponding to the model in a new molecule group.
- **Add to Molecule Group**: Create a new View window corresponding to an additional model in the current model group.

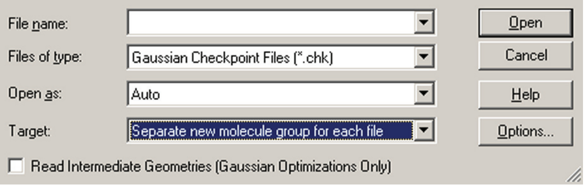
In both cases, the new View window is initially empty.



These items can also be reached via the small downward pointing triangle on the **New** button. Clicking on the **New** icon itself (avoiding the triangle's panel) selects the **Create Molecule Group** item.

## Opening Existing Models and Other Files

The **File=>Open** menu item and the **Open** button both bring up the **Open File** dialog. The format of this dialog follows the native form for the local computer, with the addition of some GaussView-specific fields which are illustrated in Figure 59.



File name:
Files of type: Gaussian Checkpoint Files (*.chk)
Open as: Auto
Target: Separate new molecule group for each file
☐ Read Intermediate Geometries (Gaussian Optimizations Only)

Figure 59. GaussView Fields in the Open File Dialog

*GaussView adds three fields and a checkbox to the standard Open File dialog provided by the operating system.*

These additional items have the following meanings. The **Files of Type** popup is used to select the file type to open. It also acts as a filter selecting which files are displayed in the dialog's file list. The file list will be limited to the files with the selected extension(s). Supported file types include:

- Gaussian Input Files (.com or .gjf)
- Gaussian Output Files (.log or .out)
- Cube Files (.cub)
- Gaussian Checkpoint Files (.chk)
- Gaussian Formatted Checkpoint Files (.fch or .fchk)
- Brookhaven PDB Files (.pdb or .pdb1)
- MDL Mol Files (.mol, .rxn or .sdf)
- Sybyl Mol2 Files (.mol2 or .ml2)
- CIF Files (.cif)

All files may also be displayed if desired by selecting the **All Files** item.

The **Open as** popup is used to force an input file to be interpreted as the specified file type, regardless of the actual file extension. All supported file types are available as choices here. The default is **Auto**, which identifies the file type by its extension alone.

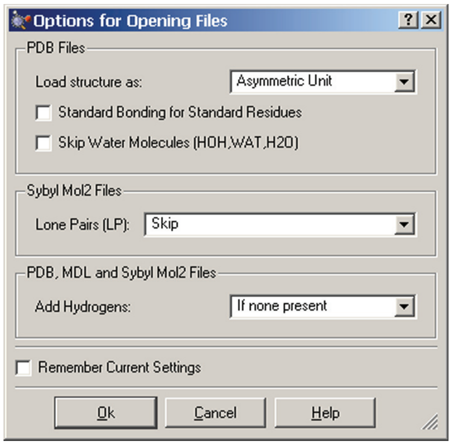
The **Target** popup specifies where the read-in structure should be placed:

- **Separate new molecule group for each file**: Create a new, one-member molecule group for each file that is read in. This is the default.
- **Single new molecule group for all files**: Create one new molecule group, and make each file a molecule within it. When opening a single file, this is equivalent to the first option.
- **Append all files to active molecule**: Place the structures from all opened files into the current molecule (in the current molecule group). This will result in additional fragments being added.
- **Add all files to active molecule group**: Add each file as a separate, new molecule within the current molecule group. The current molecule is left unchanged.
- **Add single new molecule for all files**: Add the structures from all files into a single, one-member molecule group (similar to the third option but creates a new molecule).

In general, only the first structure present in a file is input. Thus, only the structure in the first job step of Gaussian input files is retrieved. However, when selected, the **Read Intermediate Geometries (Gaussian Optimizations Only)** checkbox causes GaussView to retrieve all geometries that are present in some Gaussian results files as separate models within the designated target. This box applies to results files from geometry optimizations, IRC jobs, ADMP and BOMD trajectory calculations and potential energy surface scans: all jobs with an optimization component. It is not valid with the **Append all files to active molecule** choice.

## Additional File Open Options

Clicking on the **Options** button in the **Open File** dialog results in the dialog in Figure 60. It contains items which modify the default file opening/structure reading/processing behavior for PDB files and some related types. The settings in this dialog can be retained across uses by checking **Remember Current Settings** at the bottom left.



Options for Opening Files

PDB Files

Load structure as: Asymmetric Unit

☐ Standard Bonding for Standard Residues

☐ Skip Water Molecules (HOH,WAT,H2O)

Sybyl Mol2 Files

Lone Pairs (LP): Skip

PDB, MDL and Sybyl Mol2 Files

Add Hydrogens: If none present

☐ Remember Current Settings

**Figure 60.** File Opening Options

The following options in the first and third sections apply to PDB files:

- **Load Structure as**: Specifies handling of crystallographic structures, interpreting them as an asymmetric unit, a unit cell or a biological unit.
- **Standard Bonding for Standard Residues**: If unchecked, GaussView determines connectivity using the default distance cutoffs-based method. When checked, applies connectivity based on the contained residue specifications.
- **Skip Water Molecules**: If checked, ignores any water molecules present in the PDB file (specifically, HOH, WAT and/or H2O).
- **Add Hydrogens**: Specifies when to automatically add hydrogen atoms to the converted structure. By default, hydrogens are added when none are present in the file. The **Yes** and **No** options say to always/never add hydrogen atoms where appropriate.

The latter option also applies to MDL and Sybyl Mol2 files. The following option applies to Sybyl Mol2 files:

- **Lone Pairs (LP)**: Determines whether lone pairs are skipped or replaced with open valence atoms.

## Accessing Recent and Related Files

The **File=>Recent Files** menu path contains a list of files that have been opened most recently. You can specify the number of items in the list with the **Maximum Recent Files** field in the **File/Directory** preferences. The file list is saved across GaussView sessions.

The **File=>Related Files** menu path contains a list of openable files which are related to the active molecule (e.g., Gaussian output file, checkpoint file, and so on).

The **File=>Refresh** menu path reloads from the current molecule from its original file, centering and possibly reorienting the molecule. It is available only when the current molecule has not been modified.

## Viewing the Input File for the Current Results

Pressing the **View File** button or selecting the **Results=>View File** menu item opens the file which was opened for the current model, provided that the molecule has not been structurally modified in any way since it was opened. In the case of binary input files like Gaussian checkpoint files, the displayed file will be the one that was created automatically by GaussView with the FormChk utility.

## Saving Molecules

The **File=>Save** menu item and the **Save** button allow you to save the current model to an external file or set of files. These items use the system's **Save** dialog, to which GaussView adds some additional fields (see Figure 61).

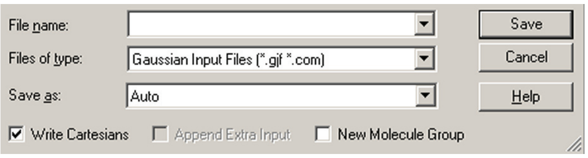

File name:
Files of type: Gaussian Input Files (*.gjf *.com)
Save as: Auto
☑ Write Cartesians ☐ Append Extra Input ☐ New Molecule Group

Figure 61. GaussView Fields in the Save File Dialog

*GaussView adds several fields to the standard system Save dialog. Molecules can be written in several formats.*

These fields have the following meanings:

- **Files of type**: Acts as a filter, selecting which files are displayed in the dialog's file list.
- **Save as**: Forces the saved file to be written as the selected type, regardless of the file extension that it is assigned. The default is **Auto**, which selects the output file format based on its extension.
- **Write Cartesians**: If checked, the molecular structure is written in Cartesian coordinates in the saved file. By default, a Z-matrix is written.
- **Append Extra Input**: This control is active for models which were read in from Gaussian input files. If there was additional input present in the file, checking this box will cause it also to be included in the output file.
- **New Molecule Group**: If checked, GaussView also creates a new molecule group containing the saved molecule.

Within a molecule group, the current model is saved. There is no way to save all of the molecules within a molecule group to a single file or to a group of files in a single operation.

# Printing and Saving Images

Various options on the **File** and **Edit** menus, along with the corresponding buttons, can be used to print the contents of view windows and to save their graphical displays as image files.

## Printing

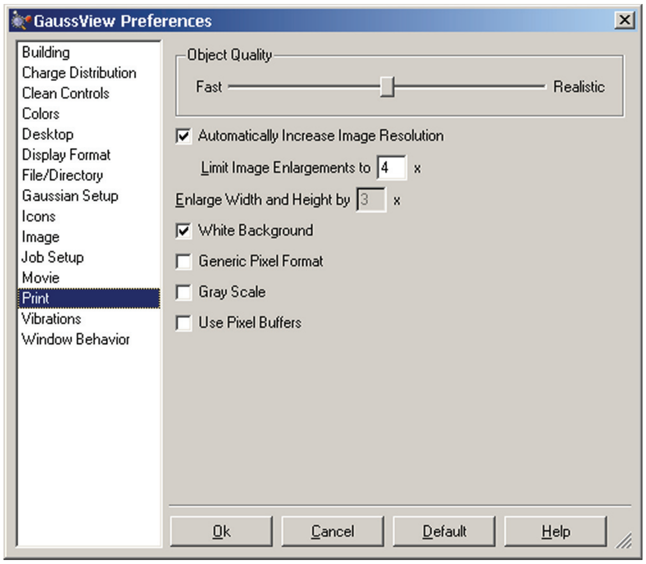
The image in the active View window can be printed by selecting **File=>Print** or clicking on the **Print** button. The normal operating system **Print** dialog is then displayed.

Print output is also controlled by settings in the **Print Preferences**, as shown in Figure 62. Settings in the **Print** dialog have precedence over those in the preferences.

The default print operation increases the image resolution to match the printer resolution, up to the maximum factor specified in the preferences, and prints the image on a white background. Note that the image always prints at its current size (despite the wording of the second control). If you need to enlarge an image, use the **Enlarge Width and Height** instead (or in addition). A color image is produced unless **Gray Scale** is selected.

The **Object Quality** slider specifies the image quality. Moving the slider toward the **Realistic** end of the scale increases the file size and the time required to generate the image file. The maximum setting is recommended for publication quality images.

The remaining controls specify low-level graphics behavior. **Generic Pixel Format** says to use the system software renderer. This option should be checked only after rendering problems/failures have been encountered during image capture or printing. **Use Pixel Buffers** says to use OpenGL pixel buffers (may improve graphics performance in some implementations).



☑ Automatically Increase Image Resolution

Limit Image Enlargements to 4 x

Enlarge Width and Height by 3 x

☑ White Background

☐ Generic Pixel Format

☐ Gray Scale

☐ Use Pixel Buffers

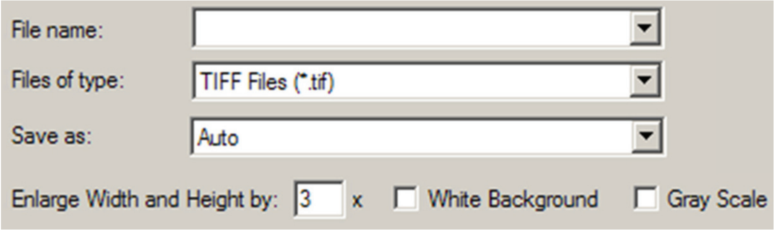
**Figure 62.** GaussView Print Preferences

*This panel allows you to specify that printed images are always enlarged to match the printer resolution (subject to the maximum value in the Limit Enlargements to field) and/or that images always appear on a white background (vs. the background used in its View window), as well as other choices.*

## Capturing Images and Saving Image Files

The **Edit=>Image Capture** menu path may be used to capture the image in the current view windows to the system clipboard (from which it may be pasted into another application). The **File=>Save Image File** menu item and the **Save Image** button allow you to save an image to an external file. They use the system Save dialog, with some additional fields as shown in Figure 63.

The **Files of type** field acts as usual as a filter determining what files are displayed in the file list. The **Save as** field specifies the kind of graphics file to be produced (by default, this is determined from file extension). The available files types are JPEG, PNG, TIFF, JPEG2, vector-based EPS, Windows Bitmap and GIF. In general, we recommend selecting TIFF for later high resolution printing and selecting JPEG or PNG for use on the web or in presentations.



File name:

Files of type: TIFF Files (*.tif)

Save as: Auto

Enlarge Width and Height by: 3 x ☐ White Background ☐ Gray Scale

**Figure 63.** GaussView Fields in the Save Image Dialog

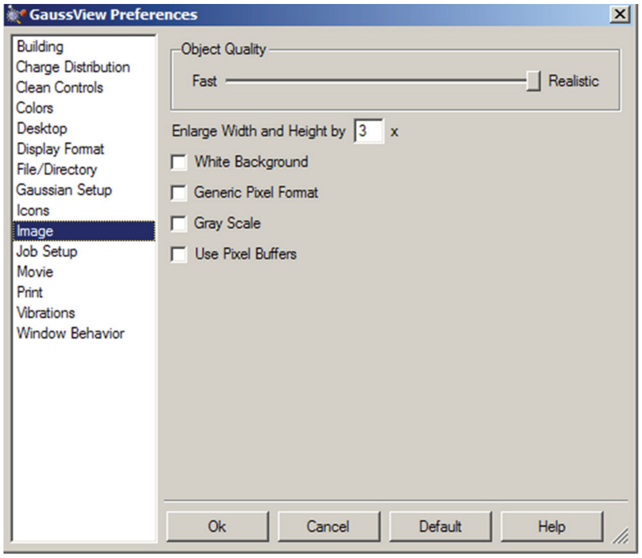
*These fields are added to the standard system Save dialog by GaussView when saving images.*

The other GaussView fields in the dialog have the following meanings:

- **Enlarge Width and Height by**: Enlarge the image by uniform scaling in order to increase its physical size and/or graphical resolution (the default value is 3x). Use a factor of 4 if you plan to ultimately print the image at 300 dpi (at its current size). If you also want to increase the image size, you must also include this factor. Thus, to save the current image at 300 dpi at twice its current size, you would use an enlargement factor of 8. Note that the computation time for rendering increases as the square of the enlargement factor.
- **White Background**: Use a white background. The background in its View window is used if this item is unchecked.
- **Use Gray Scale**: Convert the image to gray scale (black and white) before saving. The default is to save a color image.

Both image capture and image saving are subject to the settings in the **Image Preferences,** shown in Figure 64. Settings in the **Save** dialog override those in the preferences. The fields in this panel have the following meanings:

- **Object Quality**: Specifies the image quality. Moving the slider toward the **Realistic** end of the scale increases the file size and the time required to generate the image file.
- **Enlarge Width and Height by**: Set the default image scaling factor (as above).
- **White Background**: Use a white background (the default). The background in its View window is used if this item is unchecked.
- **Generic Pixel Format**: Use the system software renderer. This option should be checked only after rendering problems/failures have been encountered during image capture or printing.
- **Use Gray Scale**: Convert the image to gray scale (i.e., black and white) before capturing. The default is to save a color image.
- **Use Pixel Buffers**: Use OpenGL pixel buffers (may improve graphics performance in some implementations).



Object Quality
Fast ——— Realistic

Enlarge Width and Height by 3 x

☐ White Background

☐ Generic Pixel Format

☐ Gray Scale

☐ Use Pixel Buffers

Figure 64. Image Capture Preferences

*This panel allows you to set defaults for image captures. Preferences for Movies are similar.*

## Saving Movies

The **File=>Save Movie** menu path and the **Save Movie** button save the various frames in the current molecule group as an animation. The menu path leads to a submenu, which can also be reached by clicking on the small triangle in the button. The submenu has the following selections:

- **Save Movie File:** Save the frames as a single animation. The available formats are animated GIF and MNG.

- **Save Movie Frame Files:** Save each frame/molecule within the molecule group as a separate image file. This option is really a shortcut for saving each molecule as an individual image. It is also useful if you want to create your own animation from individual frame files in external software.
- **Save Both:** Both an animation and the individual frames are saved. You will see two save dialogs in order to specify both file types.

Clicking on the **Save Movie** icon on the button selects the **Save Movie File** choice.

The **Movie Preferences** are similar to those for Images (see Figure 64).

### Saving Plot and Spectrum Images

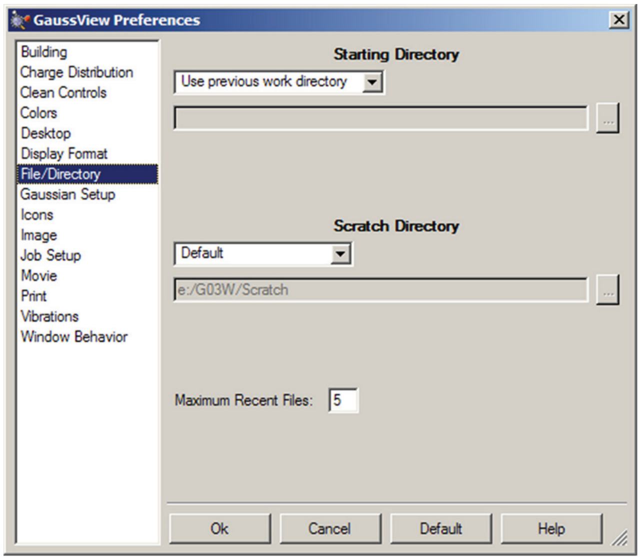
The various plots produced by GaussView are discussed in detail later in this manual. However, you can save an image file of any plot/spectrum by right-clicking anywhere within the plot area and selecting **Export** from the resulting context menu. Doing so will cause a **Save** dialog to open. You can specify the desired type of graphics file using its **Save as type** popup menu.

## Specifying Default File Locations

The **File/Directory Preferences** are illustrated in Figure 65. They allow you to specify the default locations for various kinds of GaussView-related files.

The **Starting Directory** popup allows you to select the following choices:

- **Use previous work directory**: Keep track of the last directory visited and use that directory the next time.
- **Use launch directory**: Always use the directory from which GaussView launched as the default directory.
- **Specify**: Always use the specified directory.



Starting Directory: Use previous work directory

Scratch Directory: Default

e:/G03W/Scratch

Maximum Recent Files: 5

**Figure 65. Specifying Default Directory Locations**

*This dialog allows you to specify default directory locations for file opens and saves, GaussView's scratch directory and the custom fragment library. It also specifies how many files to include in the recent file list and whether to use filename completion within dialogs (if the operating system supports it).*

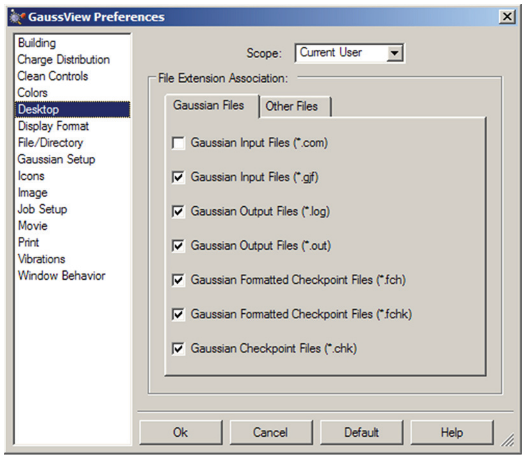
The **Scratch Directory** popup, which specifies the location for temporary scratch files that GaussView uses in some cases, has the following choices:

- **Use GAUSS_SCRDIR**: Use the Gaussian scratch directory for GaussView as well (as defined by the environment variable of this name).

- **Use launch directory**: Always use the directory from which GaussView launched as the scratch directory.
- **Specify**: Always use the specified directory as the scratch directory.

## Specifying File Associations Under Windows

On Windows systems, the **Desktop** section of the **Preferences** dialog allows you to set file associations: file extensions which will be associated with GaussView and for which the application will be opened automatically when such a file is opened. It is illustrated in Figure 66. Note that the file extensions are divided among two panels.


GaussView Preferences
Building
Charge Distribution
Clean Controls
Colors
Desktop
Display Format
File/Directory
Gaussian Setup
Icons
Image
Job Setup
Movie
Print
Vibrations
Window Behavior
Gaussian Files
Other Files
Ok
Cancel
Default
Help

Scope: Current User

File Extension Association:

☐ Gaussian Input Files (*.com)
☑ Gaussian Input Files (*.gjf)
☑ Gaussian Output Files (*.log)
☑ Gaussian Output Files (*.out)
☑ Gaussian Formatted Checkpoint Files (*.fch)
☑ Gaussian Formatted Checkpoint Files (*.fchk)
☑ Gaussian Checkpoint Files (*.chk)

**Figure 66.** Specifying Windows File Associations

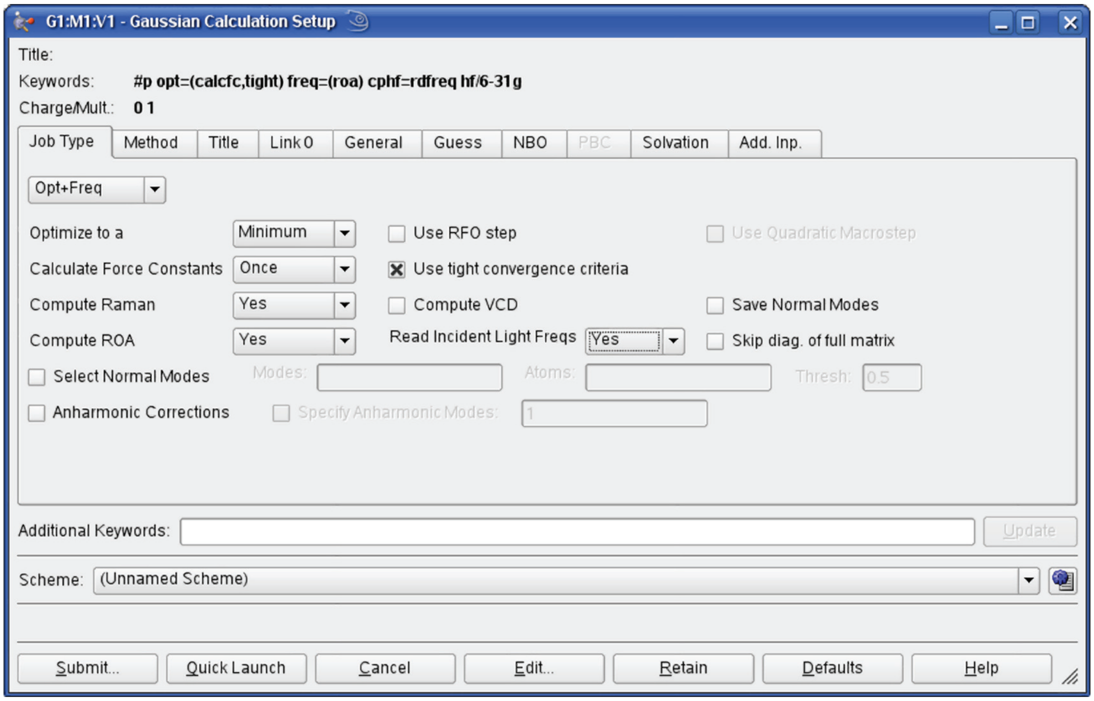
*To create a file association between GaussView and the listed Gaussian file type, place a check mark in the associated box. Removing the check mark similarly removes the file association. The Scope field specifies whether the file association is to affect only the current user or all users on the system.*

# Setting up and Running Gaussian Jobs

This chapter discusses setting up and running Gaussian calculations with GaussView. It deals only with the mechanics of doing so. Consult the *Gaussian 09 User's Reference* for detailed information about all Gaussian 09 keywords and options.

## The Gaussian Calculation Setup Window

The first step in producing a Gaussian input file is to build the desired molecule. The bond lengths, bond angles, and dihedral angles for the molecule will be used by GaussView to write a molecular structure for the calculation. Once this is completed, you can use the **Calculate=>Gaussian Calculation Setup** menu path to open the **Gaussian Calculation Setup** dialog. It is illustrated in Figure 67.



Title:
Keywords: #p opt=(calcfc,tight) freq=(roa) cphf=rdfreq hf/6-31g
Charge/Mult.: 0 1

Opt+Freq

Optimize to a: Minimum
Calculate Force Constants: Once
Compute Raman: Yes
Compute ROA: Yes
☐ Use RFO step
☒ Use tight convergence criteria
☐ Compute VCD
Read Incident Light Freqs: Yes
☐ Use Quadratic Macrostep
☐ Save Normal Modes
☐ Skip diag. of full matrix
☐ Select Normal Modes
Modes:
Atoms:
Thresh: 0.5
☐ Anharmonic Corrections
☐ Specify Anharmonic Modes: 1

Additional Keywords:
Scheme: (Unnamed Scheme)

Figure 67. The Gaussian Calculation Setup Dialog

*This dialog allows you to set up virtually all types of Gaussian calculations and to submit them from GaussView. The route section that GaussView is generating appears at the top of the dialog, and it is constantly updated as you make selections in the dialog.*

The **Gaussian Calculation Setup** dialog contains several panels, described individually below. The buttons at the bottom of the dialog have the following effects:

- Submit: Starts a Gaussian calculation using the current input file. You will be prompted to save the input file if you have not already done so.
- Quick Launch: Launches a Gaussian job without further ado (discussed later in this section).
- Cancel: Closes the dialog box and returns all selections to their default values.
- Edit: Allows direct access to the input file with an external text editor. The input file is not available for editing until it has been saved with GaussView.
- Retain: Closes the dialog box. Current selections are retained, but the input file is not created/updated, and no Gaussian job is submitted.

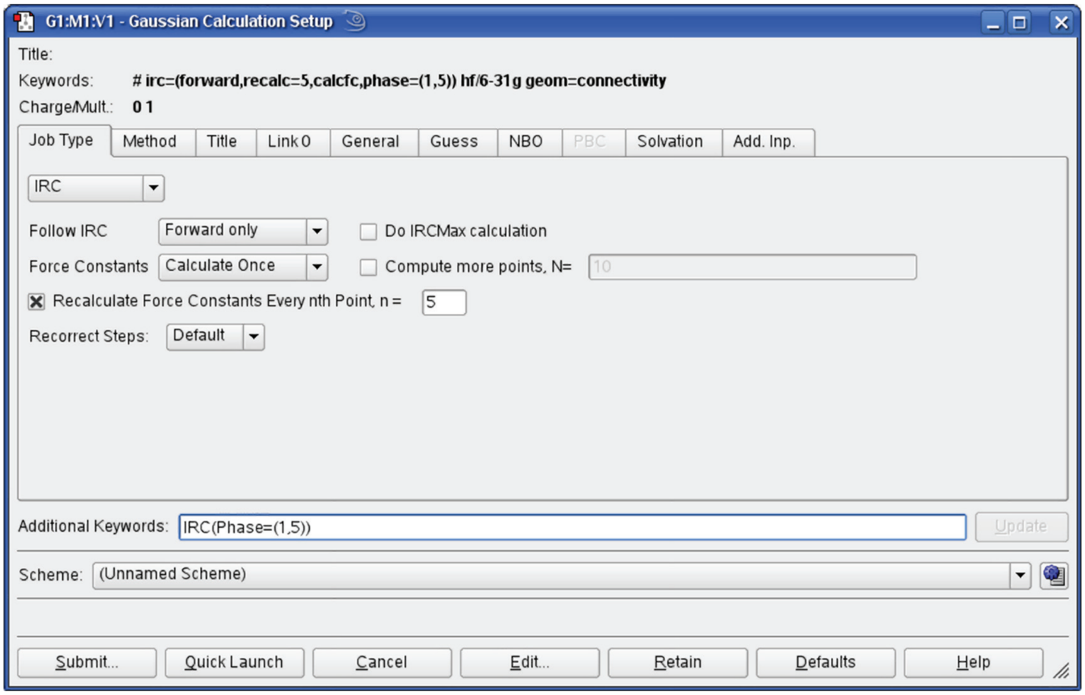
- **Defaults**: Returns all items to their default values.
- **Help**: Provides online help for this dialog.

## The Job Type Panel

The **Job Type** panel appears in Figures 67 and 68. The top popup menu selects the job type. The default is a single point energy calculation. The remaining fields in the panel represent common options for the selected job type (Figure 67 shows the ones for an **Opt+Freq** calculation).

In order to select a different job type than those listed in the popup menu, select the blank menu item at the bottom of the list, and then type the appropriate Gaussian keyword into the **Additional Keywords** section in the lower section of the dialog.

You can also use this field to add any desired Gaussian keyword and/or option. In the latter case, you must repeat the keyword within this field even if it already appears in the route section. GaussView will merge all options for the same keyword within the route section (see Figure 68 for an example). Note that this area is designed only for adding keywords to the route section. Use the **Edit** button for creating complex input files.



Title:
Keywords: # irc=(forward,recalc=5,calcfc,phase=(1,5)) hf/6-31g geom=connectivity
Charge/Mult.: 0 1

IRC
Follow IRC: Forward only
☐ Do IRCMax calculation
Force Constants: Calculate Once
☐ Compute more points, N= 10
☒ Recalculate Force Constants Every nth Point, n = 5
Recorrect Steps: Default

Additional Keywords: IRC(Phase=(1,5))
Scheme: (Unnamed Scheme)

**Figure 68. Adding an Option via the Additional Keywords Field**

*This window illustrates GaussView's ability to merge options selected from dialog controls with ones typed into the Additional Keywords field. Here, we've added the Phase option to the IRC keyword, while another option has been generated with the Calculate Force Constants popup selection.*

The **Scheme** field at the bottom of the dialog is used to quickly retrieve a stored set of keywords and options. This feature is described later in this chapter.

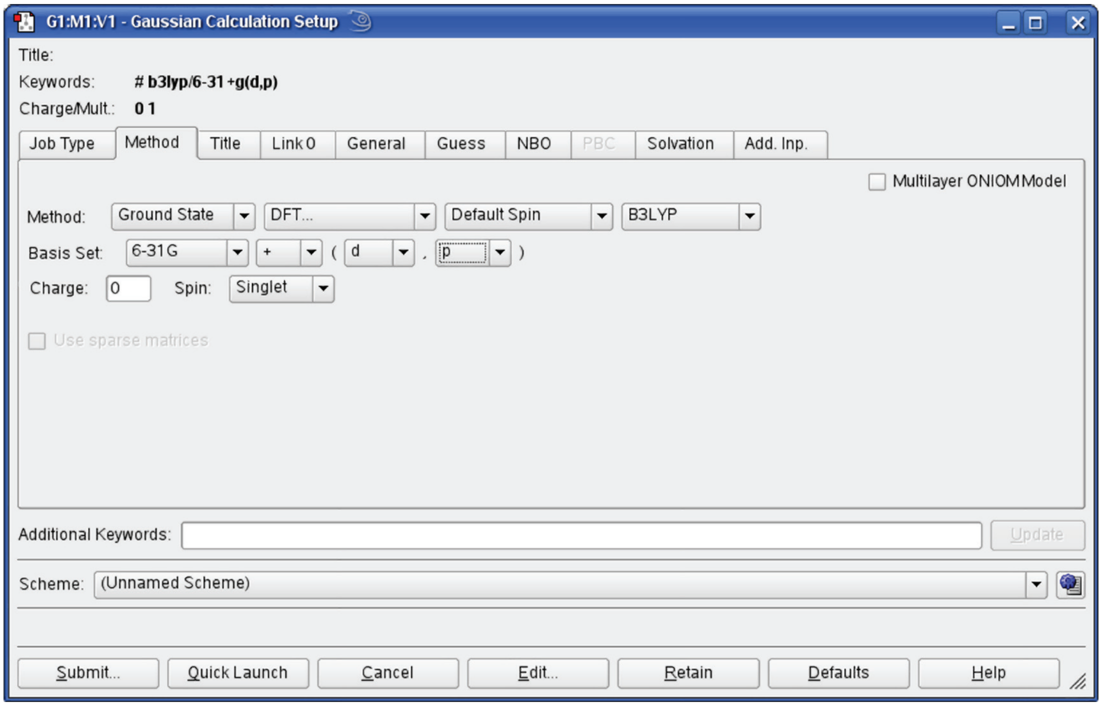
## The Method Panel

The **Method** panel specifies the quantum mechanical method to be used in a calculation. The default method is a ground state, closed shell Hartree-Fock calculation using the 3-21G basis set. This panel is illustrated in Figure 69.

The fields in the **Method** line specify the following items:

- Whether the calculation is for a ground state or an excited state.

- The theoretical method. For some choices, a fourth field is used to select the specific method of the given type. For example, in Figure 69, the method field is set to **DFT**, and the fourth field selects the B3LYP functional.
- The wavefunction type (closed shell vs. open shell). The default is an unspecified type. The **Restricted**, **Unrestricted**, and **Restricted-Open** selections prepend **R**, **U** and **RO** to the method keyword (respectively).


G1:M1:V1 - Gaussian Calculation Setup

Title:

Keywords: # b3lyp/6-31+g(d,p)

Charge/Mult.: 0 1

Method: Ground State | DFT... | Default Spin | B3LYP

Basis Set: 6-31G | + | ( d , p )

Charge: 0 Spin: Singlet

Additional Keywords:

Scheme: (Unnamed Scheme)

Figure 69. The Method Panel

*The Method panel is where the model chemistry for the calculation is specified.*

The **Basis Set** menus allow the selection of the basis set to be used in the calculation. Polarization functions and diffuse functions may be added to the basis set using the corresponding menus in this line. Select the **Custom** item at the bottom of the basis set menu to select a basis set other than those that can be constructed via the controls in this area. You may enter any basis set keyword in the name field:

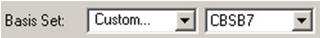

Basis Set: Custom... | CBSB7

Figure 70. Entering a Custom Basis Set Keyword

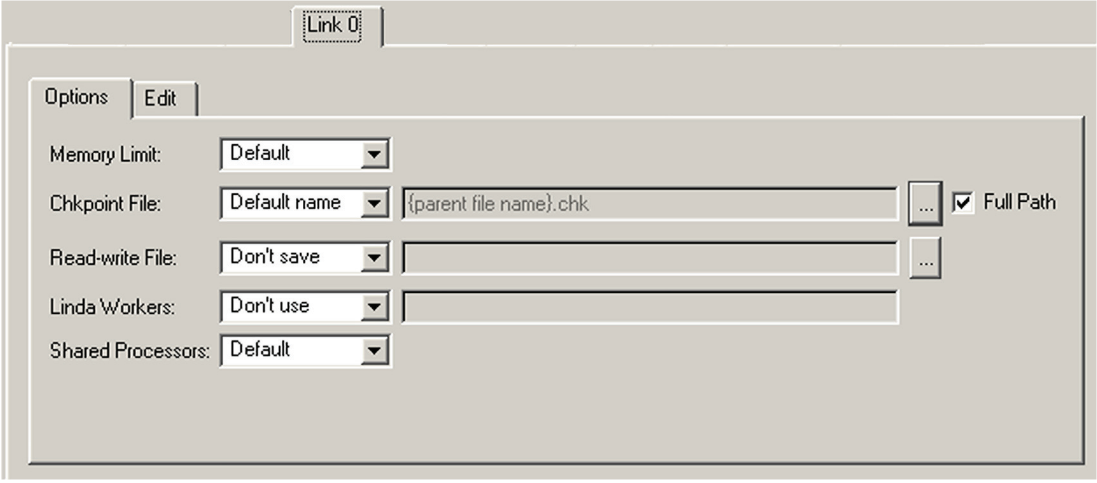
The **Charge** and **Spin** fields specify the molecule's charge and spin multiplicity. GaussView will select values for these fields based on the molecular structure. They may be modified as needed.

## The Title Panel

The **Title** panel holds a field used for the Gaussian title section (designed to contain a brief description of the job). Type your description into the text box.

## The Link 0 Panel

The **Link 0** panel is used for entering Link 0 commands for the job (see Figure 71). Note that if you remove the specification for the name and location of the checkpoint file, you will not be able to visualize output automatically from this job.



Memory Limit: Default

Chkpoint File: Default name {parent file name}.chk ☑ Full Path

Read-write File: Don't save

Linda Workers: Don't use

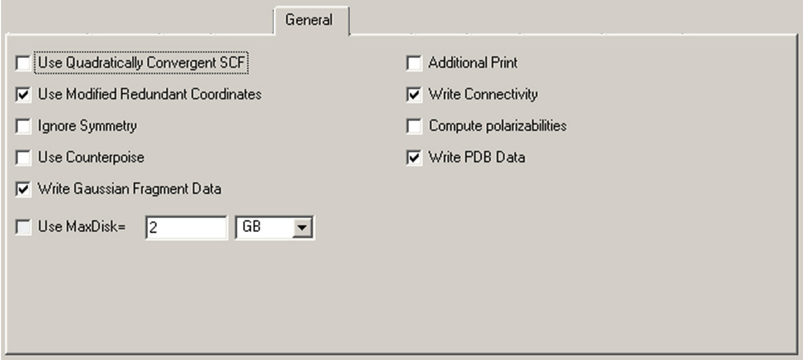
Shared Processors: Default

**Figure 71.** The Link 0 Panel

*This panel specifies a name for the checkpoint file and the read-write file, the amount of memory to use for this job, the number of shared memory processors and/or the locations of Linda workers. You can specify the various settings via controls in the Options subpanel. Alternatively, you can edit the Link 0 commands directly using the Edit subpanel. The Full Path checkbox controls whether an absolute path (checked) is used with %Chk/*

## The General Panel

The **General** panel allows you to select commonly used general calculation options. It is illustrated in Figure 72.



☐ Use Quadratically Convergent SCF

☑ Use Modified Redundant Coordinates

☐ Ignore Symmetry

☐ Use Counterpoise

☑ Write Gaussian Fragment Data

☐ Use MaxDisk= 2 GB

☐ Additional Print

☑ Write Connectivity

☐ Compute polarizabilities

☑ Write PDB Data

**Figure 72.** Selecting General Gaussian Options

*This panel contains a set of commonly used options. This window illustrates the defaults.*

The following table indicates the Gaussian keywords corresponding to these items:

| Option | Default | Keyword |
|---|---|---|
| **Use Quadratically Convergent SCF** | Off | **SCF=QC** |
| **Use Modified Redundant Coordinates** | On | **Geom=ModRedundant** |
| **Ignore Symmetry** | Off | **NoSymm** |
| **Use Counterpoise** | Off | **Counterpoise** |
| **Write Gaussian Fragment Data** | On | **Fragment** (in molecule specification) |
| **Use MaxDisk=** | Off | **MaxDisk** |
| **Additional Print** | Off | **#P** |
| **Write Connectivity** | On | **Geom=Connectivity** |
| **Compute polarizabilities** | Off | **Polar** |
| **Write PDB Data** | On | **ResNum**, **ResName**, **PDBName** (in molecule specification) |

The **Use Modified Redundant Coordinates** item is enabled only if you have set up redundant coordinates with the Redundant Coordinate Editor. If not, the item is ignored (despite its default value). **Write Gaussian Fragment Data** and **Write PDB Data** are enabled by default, but have no effect unless the corresponding items are defined.

The **Write Connectivity** option also includes the appropriate additional input section(s) in the Gaussian input file.

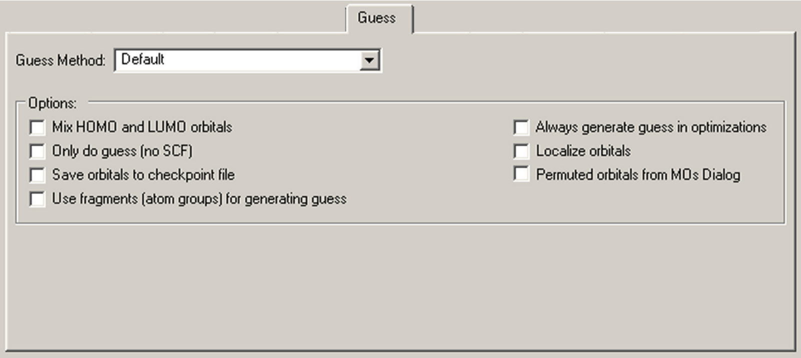
*Note*: Consult the discussion of the **SCF** keyword in the *Gaussian 09 User's Reference* for recommendations for unusual/problem cases (**SCF=QC** is not always the best next choice).

## The Guess Panel

The Guess panel contains settings related to the initial guess. It is illustrated in Figure 73. Consult the discussion of the Guess keyword in the *Gaussian 09 User's Reference* for full details on these options.

The **Guess Method** popup specifies the type of initial guess to use. It has the following options:

- **Default**: Uses the default Harris initial guess.
- **Core Hamiltonian**: Uses the Gaussian 98 default initial guess (**Guess=INDO**). Generally, we do not recomment its use except when recommended by Gaussian, Inc. technical support staff.
- **Extended Huckel**: Uses the Huckel guess (Guess=Huckel).
- **Read checkpoint file**: Retrieves the initial guess from the checkpoint file (Guess=Read).
- **Read checkpoint; otherwise generate**: Check checkpoint file for the initial guess; generate if not present (Guess=TCheck).
- **Read input checkpoint file**: Read the guess from the checkpoint file whose name is specified in the input stream (**Guess=Input**).



Guess Method: Default

Options:

☐ Mix HOMO and LUMO orbitals
☐ Only do guess (no SCF)
☐ Save orbitals to checkpoint file
☐ Use fragments (atom groups) for generating guess
☐ Always generate guess in optimizations
☐ Localize orbitals
☐ Permuted orbitals from MOs Dialog

**Figure 73. Gaussian Initial Guess Options**
*This window shows the default settings for the initial guess.*

The options in this panel have the following meanings:

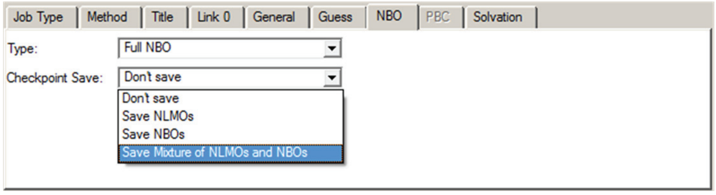
| Option | Default | Keyword |
|---|---|---|
| Mix HOMO & LUMO orbitals | Off | Guess=Mix |
| Only do guess (no SCF) | Off | Guess=Only |
| Save orbitals to checkpoint file | Off | Guess=Save |
| Use fragments (atom groups) for generating guess | Off | Guess=Fragment |
| Always generate guess in optimizations | Off | Guess=Always |
| Localize orbitals | Off | Guess=Local |
| Permuted orbitals from MOs Dialog | On | Guess=Permute |

The **Permuted orbitals for MOs Dialog** is disabled unless you have specified an alternate orbital ordering with the **MO Editor**. If enabled, it is on by default.

The **Use fragments (atom groups) for generating guess** is disabled unless fragments have been defined using the **Atom Group Editor**. If enabled, it is checked by default. In addition, fragment-specific charges and spin multiplicities are generated and placed into the route section. You can also modify them using the **Atom Group Editor** (see the example for antiferromagnetic coupling in a later section of this manual).

## The NBO Panel

The **NBO** panel is used to select NBO analysis at the conclusion of the Gaussian job. It is illustrated in Figure 74. The **Type** menu specifies the kind of NBO analysis to perform. The **Checkpoint Save** field allows you to save NBOs and/or NLMOs in the checkpoint file for later visualization (the default is **Don't Save**).



Type: Full NBO

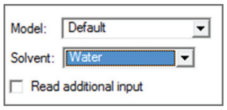
Checkpoint Save: Don't save

Figure 74. The NBO Panel

*The panel specifies the type of NBO analysis and which NBOs to save in the checkpoint file. The selection in this window is often a useful one when you will use them to generate an active space for a CASSCF calculation.*

## The Solvation Panel

The **Solvation** panel allows you to specify that the calculation is to be performed in solution rather than in the gas phase. It is illustrated in Figure 75. The **Model** field allows you to specify a specific solvation model (the default is PCM, which itself defaults to IEFPCM). You can also specify the solvent by selecting it from the corresponding popup menu. Use the **Other** selection to select a solvent other than those on the list; you will need to specify within the route section manually (e.g., placing **SCRF(EPS=***value***)** within the **Additional Keywords** field).



Model: Default

Solvent: Water

☐ Read additional input

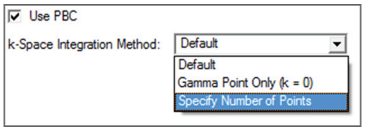
Figure 75. The Solvation Panel

*This panel specifies the SCRF model to use for solvent effects. The Default selection corresponds to the Gaussian default of SCRF=PCM.*

Note that some solvation models may present different/additional fields for their required parameters. You may use the **Read additional input** box to generate the **SCRF=Read** option; additional input may be entered using the **Add. Inp.** panel (see below).

## The PBC Panel

The **PBC** panel is used to specify options to the Gaussian **PBC** keyword (see Figure 68). Checking the **Use PBC** box causes the translation vectors to be added to the molecule specification. This is the default when a unit cell has been defined with the **Crystal Editor**. The panel is disabled for non-periodic systems.



☑ Use PBC

k-Space Integration Method: Default

Figure 76. The PBC Panel

*The Use PBC checkbox causes the translation vectors to be placed in the molecule specification. After you select the option above, an additional field for specifying the number of K-points will appear.*

### The Additional Input Panel

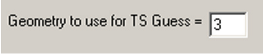
The final panel in the **Gaussian Calculation Setup** dialog is labeled **Add. Inp.** It may be used to enter any additional input section(s) required by the calculation you plan to run. This input will be written to the Gaussian input file provided that **Append Extra Input** is checked in the **Save** dialog. Any additional input present in input files that you open will also appear in this panel.

## Special Considerations for Various Gaussian Job Types

This section summarizes information about setting up various Gaussian job types for which some special steps are required. All GaussView features mentioned are discussed in detail earlier in this book.

### Transition Structure Optimizations: Opt=QST2 and Opt=QST3

Gaussian STQN-based transition structure optimizations require two or three structures as input. To set up these jobs, you must create a molecule group containing the required number of structures. If you plan on running an Opt=QST3 job, then the transition structure initial guess is assumed to be molecule 3 unless you specify a different structure on the **Job Type** panel.



Geometry to use for TS Guess = 3

Once you have done so, the **TS (QST2)** and **TS (QST3)** options will be enabled in the **Optimize to a** field for the **Optimization** job type in the Job panel of the Gaussian Calculation Setup dialog.

#### Verifying and Specifying Atom Equivalences

In most cases, GaussView will automatically identify the corresponding atoms in the multiple structures for these transition state optimizations. However, you can verify this using the **Connection Editor**, accessed via the **Connection Editor** button on the toolbar or the **Edit=>Connection Editor** menu item.

### Calculations on Polymers, Surfaces and Crystals

You can set up jobs for Gaussian's Periodic Boundary Conditions facility using the **Crystal Editor** (reached via the **Crystal Editor** button or the **Edit=>PBC** menu path). Once you have defined a unit cell, GaussView automatically sets up PBC jobs for this structure by including the translation vectors within the molecule specification. This is indicated by the enabling of the **PBC** panel in the **Gaussian Calculation Setup** dialog, and the checked **Use PBC** item. Note that for normal cases, you do not need to access this panel at all and can proceed directly to setting up Gaussian input in the normal manner.

### Multi-Layer ONIOM Calculations

GaussView contains several features for setting up ONIOM calculations.

#### Assigning Atoms to Layers

The **Layer Editor** allows you to graphically assign atoms to various ONIOM layers. It is accessed via the toolbar's **Select Layer** button or via the **Edit=>Select Layer** menu item.

#### Assigning Molecular Mechanics Atoms Types

GaussView will assign Molecular Mechanics atoms types for UFF, Dreiding and Amber (including Amber charges) to all atoms in the molecule automatically. You can view and modify these using the **Atom List Editor** (reached via the **Atom List Editor** button on the toolbar or the **Edit=>Atom List** menu path).

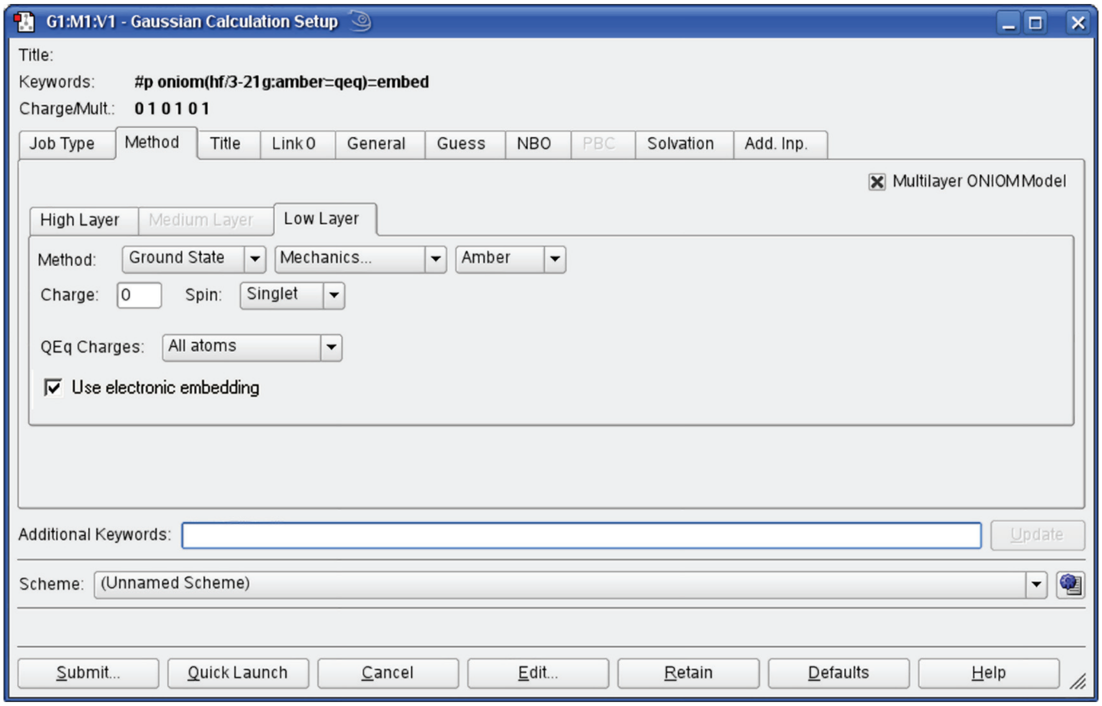
#### Defining Link Atoms

GaussView will automatically assign minimal link atom information for the appropriate atoms in an ONIOM calculation. However, all link atoms are always handled in the same way, and they may require modification for your purposes. Link atoms generated by GaussView are always hydrogens (using the H_ UFF and Dreiding atom types and the H*R* Amber atom type, where *R* is the element of the linked-to atom). The only other link atom parameter which is included is the linked-to atom (the atom in the higher layer to which the current atom is bonded); all other parameters are left blank.

The **Atom List Editor** is often a convenient way to examine and modify link atoms for ONIOM calculations. You can use the **ONIOM Layers** button to view and modify link atoms easily.

### Specifying the Model Chemistry for Each Layer

Once you have prepared the structure and specified all necessary parameters, you can set up an ONIOM calculation via the **Method** panel of the **Gaussian Calculation Setup** dialog. The **Multilayer ONIOM Model** checkbox indicates that this will be an ONIOM calculation (see Figure 77).



Title:
Keywords: #p oniom(hf/3-21g:amber=qeq)=embed
Charge/Mult.: 0 1 0 1 0 1

☒ Multilayer ONIOM Model

Method: Ground State, Mechanics..., Amber
Charge: 0
Spin: Singlet
QEq Charges: All atoms
☑ Use electronic embedding

Additional Keywords:
Scheme: (Unnamed Scheme)

**Figure 77. Setting Up a Gaussian Input File for an ONIOM Job**

*This example is preparing an input file for a two-layer ONIOM calculation. When Multilayer ONIOM Model is checked, the additional tabs appear in the Method panel. Each of them allows you to specify the theoretical method and basis set for the corresponding layer. In this case, we are using the Amber Molecular Mechanics method for the Low layer. Note that electronic embedding is requested by checking the final item in the Low Layer panel.*

## Specifying CASSCF Active Spaces Using Guess=Permute

GaussView can make it easy to specify CASSCF active space. The **MOs** dialog allows you to generate, view, select and reorder the starting orbitals. It is reached with the **Edit=>MO** Editor menu path and via the **MO Editor** button on the toolbar. See the detailed discussion of this tool earlier in this manual.

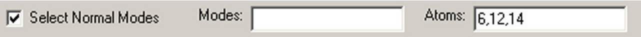
## Modifying Redundant Internal Coordinates (Geom=ModRedundant)

You can specify additions and other modifications to redundant internal coordinates for geometry optimizations and other jobs by using the **Redundant Coordinate Editor**, reached via the **Redundant Coordinate Editor** button on the toolbar or the **Edit=>Redundant Coordinates** menu path. See the detailed discussion of this tool earlier in this manual.

## Freezing Atoms During Geometry Optimizations

The **Atom Group Editor** can be used to specify atoms whose positions are to be held fixed during a geometry optimization via its **Freeze Atoms** group class. This class is defined with four groups by default, corresponding to unfrozen atoms, frozen atoms, and the first two ONIOM frozen rigid blocks (freeze settings of **-2** and **-3**; see the discussion of the **Geom** keyword in the *Gaussian 09 User's Reference* for full details on specifying frozen atoms and rigid blocks for ONIOM calculations). In order to hold specific atoms fixed during a geometry optimizations, add them to the **Freeze (Yes)** group in the **Atom Group Editor**.

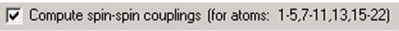
## Selecting Normal Modes for Frequency Calculations (Freq=SelectNormalModes)



☑ Select Normal Modes  Modes:  Atoms: 6,12,14

You can use the **Atom Group Editor** to select atoms for which normal mode analysis is conducted (see the *Gaussian 09 User's Reference* for details). Placing the desired atoms into the **Select Normal Modes (Yes)** group will cause them to be entered into the **Atoms** field corresponding to **Select Normal Modes** in the **Gaussian Calculation Setup**'s **Job Type** panel for **Frequency** jobs. You can modify this list as needed, but doing so will have no effect on the definition of the groups in the **Atom Group Editor**'s **Select Normal Modes** group class.

## Calculating NMR Spin-Spin Coupling (NMR=(SpinSpin,ReadAtoms))

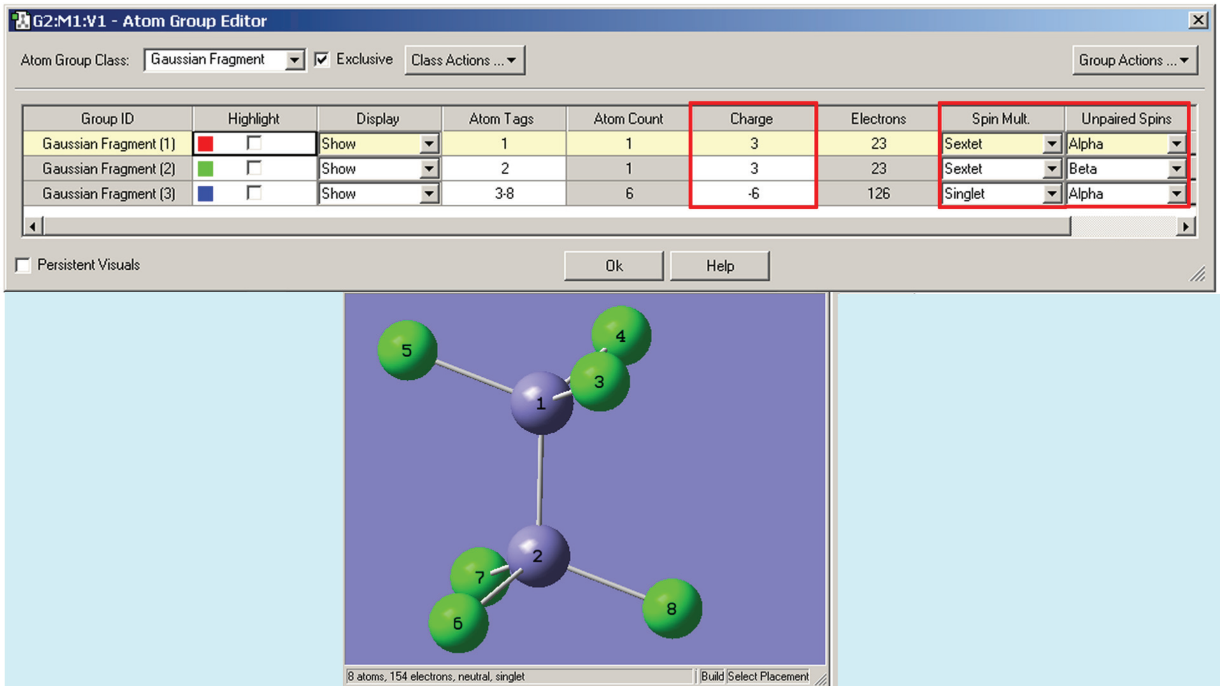


☑ Compute spin-spin couplings (for atoms: 1-5,7-11,13,15-22)

When you select an NMR calculation in the **Gaussian Calculation Setup**'s **Job Type** panel, the field to the left appears. The atom list in the parentheses corresponds to the members of the **NMR Spin-Spin (Yes)** group, as defined in the **Atom Group Editor** (by default, all atoms are placed into this group and the list of atoms reads **all atoms**). A specific group of atoms appears in this item when the **NMR Spin-Spin (No)** group contains at least one atom.

## Specifying Fragment-Specific Charges and Spin Multiplicities

You can specify individual charge and spin multiplicity values for each fragment defined via the **Atom Group Editor**. This facility is useful for setting up fragment guess jobs (**Guess=Fragment**) for modeling antiferromagnetic coupling, counterpoise calculations (**Counterpoise**) for computing counterpoise corrections and basis set superposition errors, and the like. Figure 78 illustrates setting up a system for modeling antiferromagnetic coupling effects.



| Group ID | Highlight | Display | Atom Tags | Atom Count | Charge | Electrons | Spin Mult. | Unpaired Spins |
|---|---|---|---|---|---|---|---|---|
| Gaussian Fragment (1) | 🟥 ☐ | Show | 1 | 1 | 3 | 23 | Sextet | Alpha |
| Gaussian Fragment (2) | 🟩 ☐ | Show | 2 | 1 | 3 | 23 | Sextet | Beta |
| Gaussian Fragment (3) | 🟦 ☐ | Show | 3-8 | 6 | -6 | 126 | Singlet | Alpha |

8 atoms, 154 electrons, neutral, singlet

**Figure 78. Specifying Per-Fragment Charge and Spin**

*Antiferromagnetic coupling is an effect that is important for molecules with high spin multiplicity. This Fe2Cl6 compound is a simple example. Here, we have defined three fragments. Each iron atom is in its own fragment, and the six chlorine atoms are in a third fragment. The two iron fragments are each assigned a charge of +3, and both are defined as sextets with opposite spin (i.e., spin multiplicities of 6 and -6). The fragment containing the chlorine atoms is defined as a singlet with a -6 charge. These values will be placed into the route section of the Gaussian job set up in GaussView.*

The **Gaussian Calculation Setup**'s **General** panel contains features relevant to these two calculation types: **Write Gaussian Fragment Data** (for both types) and **Use Counterpoise** (for **Counterpoise** calculations). In addition, the **Guess** panel has two items useful for the first job step of a fragment guess job: **Only do Guess (no SCF)** and **Use fragments (atom groups) for generating guess**, corresponding to **Guess=Only** and **Guess=Fragment** (respectively). Typically, such a job would be followed by a second job to compute the energy including the antiferromagnetic coupling: **Guess=Read Geom=AllCheck Stable=Opt**.

## Setting Defaults for Gaussian Jobs

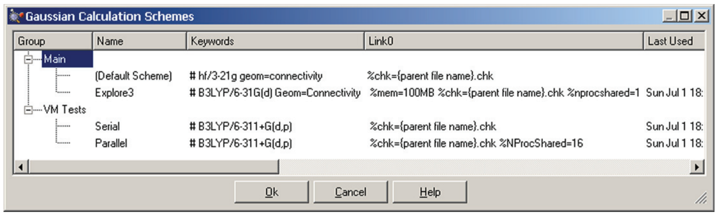
The **Gaussian Setup Preferences** may be used to specify defaults for the **Gaussian Calculation Setup** dialog. Click the **Calculation** button, and then specify the desired settings for future Gaussian calculations. These will be applied to future job setup operations.

### Defining Calculation Schemes

Modifying the **Gaussian Setup Preference**s as described in the preceding paragraph has the effect of modifying the Gaussian calculation scheme named **Default**. Schemes are named sets of calculation keywords and options, and you can define and save as many different ones as you want to. You can view the calculation scheme in effect at the bottom of the **Gaussian Calculation Setup** dialog and in the scheme popup in the toolbar, and in the **Calculate=>Gaussian Calculation Scheme** submenu. You can apply a scheme to the current molecule using any of these controls as well.

For new molecules, the **Default** scheme is initially applied. When you open a new molecule from a file, the scheme will be set to the scheme that matches its settings (if any) or to **Unnamed Scheme**.

You can view and modify the properties of the various defined schemes using the **Schemes** button or by selecting **More Schemes** from any scheme list. The resulting dialog appears in Figure 79.



| Group | Name | Keywords | Link0 | Last Used |
|---|---|---|---|---|
| Main | | | | |
| | (Default Scheme) | # hf/3-21g geom=connectivity | %chk={parent file name}.chk | |
| | Explore3 | # B3LYP/6-31G(d) Geom=Connectivity | %mem=100MB %chk={parent file name}.chk %nprocshared=1 | Sun Jul 1 18: |
| VM Tests | | | | |
| | Serial | # B3LYP/6-311+G(d,p) | %chk={parent file name}.chk | Sun Jul 1 18: |
| | Parallel | # B3LYP/6-311+G(d,p) | %chk={parent file name}.chk %NProcShared=16 | Sun Jul 1 18: |

Figure 79. Viewing and Modifying Calculation Schemes
*This dialog shows four schemes organized into two groups.*

Any field within a scheme can be edited by clicking on it. Right clicking on a scheme produces a context menu, allowing you to add groups and schemes, cut and paste between fields, and delete schemes. You can also save schemes to an external file and load ones saved in this way back into GaussView. Note that neither the **Default** scheme nor the **Main** group may be renamed or deleted.

## The Quick Launch Feature

The conventional way to run a Gaussian job from GaussView is to open the **Gaussian Calculation Setup**, set the correct job options, click the **Submit** button, and specify the name and location for the input file. The Quick Launch feature greatly simplifies this common task. A job can be launched using the **Quick Launch** toolbar button, the **Quick Launch** button in the **Gaussian Calculation Setup** dialog or the **Calculate=>Gaussian Quick Launch** menu path.

Clicking on the button in the **Gaussian Calculation Setup** dialog or on the portion of the toolbar icon to the left of the small arrow will immediately launch a Gaussian job using the current calculation scheme and temporary files. The toolbar icon arrow and the **Calculate** menu item both lead to a submenu. Its **Temp File** item will also result in a job started from a temporary input file. The **Save File** option will prompt you to save an input file and submit that file as a Gaussian job afterwards. Finally, the **Save and Edit File** option will prompt you to save an input file and then open that file in the external editor.

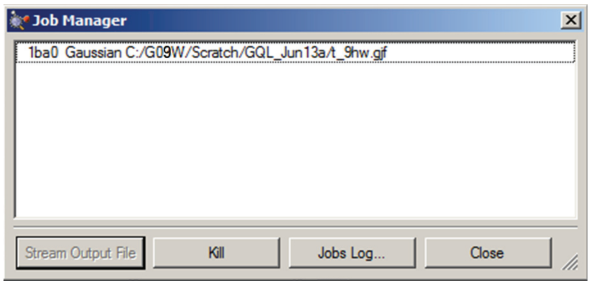
When you start a new calculation using Quick Launch a new View window is opened corresponding to it. While the job is running, a text message identifying the job, a stop button, and a stream output file button are placed in the status bar of the View window. Once the job finishes successfully, the results file is opened automatically in the same View window. When more than one results file is produced by a calculation—e.g., both a log file and a checkpoint file are created—then you will be prompted to select the file to open.

You can save the files generated from a Quick Launch operation to temporary files using the **File=>Save Temp Files** menu item. This item replaces the usual **Related Files** option under these circumstances.

## Viewing and Controlling Gaussian Jobs

The **Calculate=>Current Jobs** menu path opens the **Job Manager** dialog (shown in Figure 80); the **Job Manager** button on the toolbar performs the same function.

This window displays all the jobs started by GaussView that are currently running. Note that only jobs started during the current session of GaussView can be displayed. Examples of jobs that may be displayed are Gaussian jobs submitted from the Gaussian dialog box, Gaussian input file edit sessions launched from GaussView, CubeGen processes for building surfaces for display, FreqChk processes to generate vibrational analysis data, and/or processes from other Gaussian utilities.



1ba0 Gaussian C:/G09W/Scratch/GQL_Jun13a/t_9hw.gjf

**Figure 80.** The Job Manager Dialog

*This dialog allows you to view and control Gaussian jobs as well as jobs running Gaussian utilities like CubeGen. You can terminate a job using the Kill button.*

Clicking on the **Jobs Log** button displays the current GaussView job log containing system messages associated with the execution of GaussView external processes. The **Clear** button in the resulting window removes old jobs from the job list, and the **Close** button dismisses the job list window.

Note that the **Jobs Log** button does not display the log file associated with a running Gaussian job. The latter is accomplished by the **Stream Output File** button for Gaussian calculations. Note that selecting this button for job types (e.g., cube generation jobs) will display whatever file GaussView can find that is associated with the job (often the Gaussian input file).

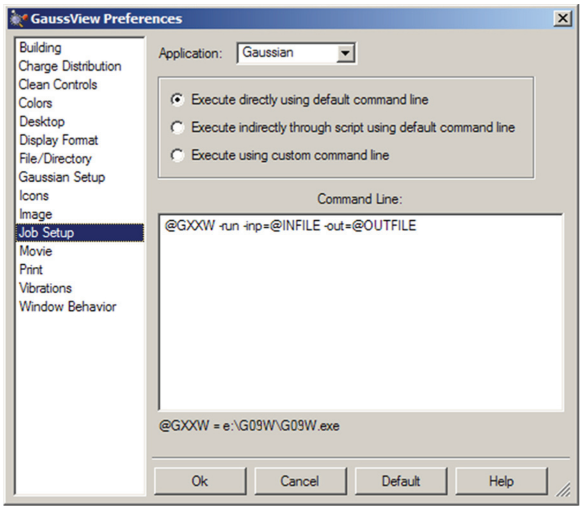
Individual jobs may be aborted using the **Kill** button.

## Specifying How the Gaussian Program is Executed

The **Job Setup Preferences** dialog allows you to examine and customize how Gaussian and its utilities are launched from within GaussView. It is illustrated in Figure 81. The **Application** field at the top of the panel specifies the program or utility whose execution method is currently displayed. Below this popup, there are three launch choices, and the command line associated with the selected launch method is displayed in the **Command Line** area (where it can also be modified).

For each job type, there are three launch choices:

- **Execute directly using default command line**: The job will be started using the command line specified in the lower area.
- **Execute indirectly through script using default command line**: The job will be started using a GaussView-provided script. These scripts are located in the bin subdirectory of the GaussView installation directory. Their names are listed below. The associated command line appears in the lower area of the dialog.
- **Execute using custom command line**: Use the command line specified in the box to start the job. You can enter whatever command line is appropriate for your situation. The GaussView provided scripts may be called if desired.



Application: Gaussian

● Execute directly using default command line
○ Execute indirectly through script using default command line
○ Execute using custom command line

Command Line:

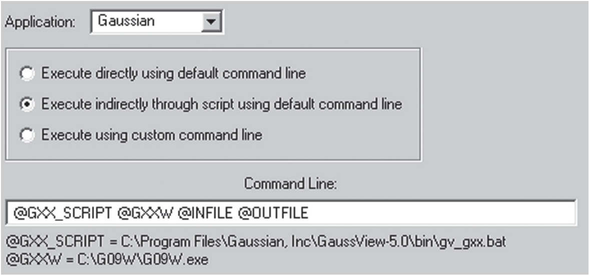
```
@GXXW -run -inp=@INFILE -out=@OUTFILE
```

@GXXW = e:\G09W\G09W.exe

Figure 81. Job Setup Preferences

*These settings are used to specify how various external jobs get initiated by GaussView.*

The following figure illustrates the command line and other information displayed for running the Gaussian program using the second launch choice:



Application: Gaussian

○ Execute directly using default command line
● Execute indirectly through script using default command line
○ Execute using custom command line

Command Line:

```
@GXX_SCRIPT @GXXW @INFILE @OUTFILE
```

@GXX_SCRIPT = C:\Program Files\Gaussian, Inc\GaussView-5.0\bin\gv_gxx.bat
@GXXW = C:\G09W\G09W.exe

Figure 82. Running Gaussian via a Script

*The Command Line field displays the command which will be used to run Gaussian via an external script (field's height is greatly reduced). The values of the GaussView internal variables used in the command line are displayed below the field for your convenience.*

GaussView provides the following scripts in its bin subdirectory:

| Menu Item | Linux/UNIX | Windows | Mac OS X |
|---|---|---|---|
| **Gaussian** | gv_gxx.csh | gv_gxx.bat | gv_gxx.csh |
| **Cubegen** | gv_cubegen.csh | gv_cubegen.bat | gv_cubegen.csh |
| **Cubman** | gv_cubman.csh | gv_cubman.bat | gv_cubman.csh |
| **FormChk** | gv_formchk.csh | gv_formchk.bat | gv_formchk.csh |

| Menu Item | Linux/UNIX | Windows | Mac OS X |
|---|---|---|---|
| **FreqChk** | gv_freqchk.csh | gv_freqchk.bat | gv_freqchk.csh |
| **Gaussian Help** | gv_gaussianhelp.csh | gv_gaussianhelp.bat | gv_gaussianhelp_mac.csh |
| **File Editor** | gv_fileeditor.csh | gv_fileeditor.bat | gv_fileeditor_mac.csh |

Each script's usage is documented in comments at the beginning of the file. Prudence dictates making a backup copy of any script before modifying it in any way. Note that all standard UNIX scripts are also provided on Mac OS X systems for your convenience.

You can specify a custom command line for external jobs using the third choice in the **Job Setup Preferences** dialog. However, successfully using this feature depends on a clear understanding of the command line invocation of Gaussian and its utilities under the current operating system. Consult the *Gaussian 09 User's Reference* for details.

The following GaussView internal variables can be used within commands. Note that they are not operating system environment variables, despite their resemblance to them in naming conventions.

| Parameter | Meaning |
|---|---|
| $GEXE | Path to the Gaussian executable (UNIX) |
| $GEXE_WIN | Path to Gaussian executable (Windows) |
| $CUBEGEN | Path to the CubeGen executable |
| $FORMCHK | Path to the FormChk executable |
| $FREQCHK | Path to the FreqChk executable |
| $MM | Path to the Gaussian MM executable |
| $WORDPAD | Path to Wordpad (Windows) |
| $NEDIT | Path to UNIX editor |
| $GHELP | Path to the GHelp executable |
| $*utilname*_SCRIPT | Path to the script for the specified utility |
| $INFILE | Gaussian input file |
| $OUTFILE | Gaussian or utility output file |
| $KIND | Type of cube for CubeGen |
| $NPTS | Cube density for CubeGen |
| $HEADER | CubeGen header flag |

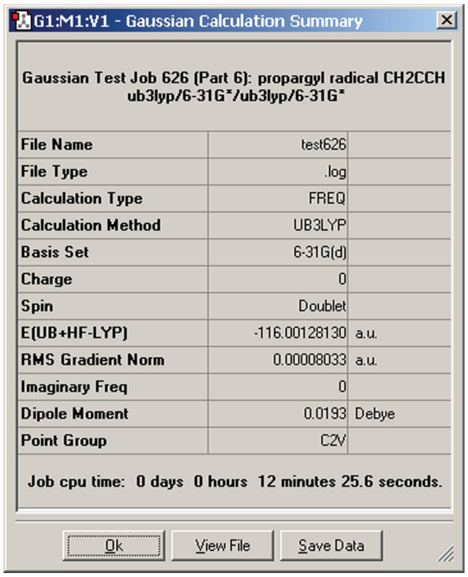
# Viewing Gaussian Results

This section describes the **Results** menu and the options available through it. This menu opens a series of dialog boxes that allow you to examine the results of calculations from Gaussian output files. If the selected item is not present in the file, the item is dimmed in the menu.

The various spectra and plots produced by GaussView can all be customized and manipulated using common techniques. These procedures are discussed in the final part of this section of the manual.

## Calculation Summary

The **Results=>Summary** menu item displays summary data about the results of the Gaussian calculation (available when a Gaussian log file or checkpoint file is opened). It is displayed in Figure 83.



Gaussian Test Job 626 (Part 6): propargyl radical CH2CCH
ub3lyp/6-31G*/ub3lyp/6-31G*

| | | |
|---|---|---|
| File Name | test626 | |
| File Type | .log | |
| Calculation Type | FREQ | |
| Calculation Method | UB3LYP | |
| Basis Set | 6-31G(d) | |
| Charge | 0 | |
| Spin | Doublet | |
| E(UB+HF-LYP) | -116.00128130 | a.u. |
| RMS Gradient Norm | 0.00008033 | a.u. |
| Imaginary Freq | 0 | |
| Dipole Moment | 0.0193 | Debye |
| Point Group | C2V | |

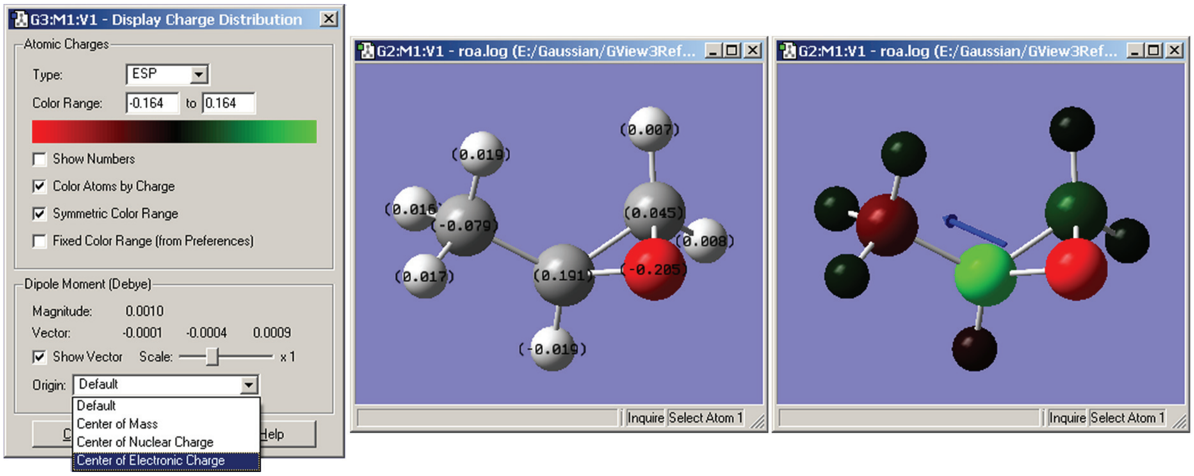
Job cpu time: 0 days 0 hours 12 minutes 25.6 seconds.

Figure 83. Summary of a Gaussian Calculation
*This window summarizes the results of a B3LYP/6-31G(d) frequency calculation.*

The **Results=>View File** menu item and the **View File** button can both be used to open the Gaussian log file associated with the Gaussian calculation (if applicable).

## Displaying Atomic Charges Computed in Gaussian

The **Results=>Charge Distribution** menu item opens the **Display Atomic Charges** dialog (see Figure 84). This tool manages the display of partial charge density as computed by various methods in Gaussian. Displays are available for the default Mulliken charges and other computed charges that are available for this job. The **Charge Type** menu lists the available choices.



G3:M1:V1 - Display Charge Distribution

Atomic Charges

Type: ESP

Color Range: -0.164 to 0.164

☐ Show Numbers

☑ Color Atoms by Charge

☑ Symmetric Color Range

☐ Fixed Color Range (from Preferences)

Dipole Moment (Debye)

Magnitude: 0.0010

Vector: -0.0001 -0.0004 0.0009

☑ Show Vector Scale: x 1

Origin: Default

Figure 84. Displaying Atomic Charges

*The dialog on the left is used to control what charges are shown and how they are displayed. The window in the middle shows the numeric charge numbers display, and the one on the right shows the atoms colored by charge (reflecting the settings in the dialog on the left), as well as the dipole moment vector.*

By default, the color spectrum for charge display is set by reading the maximum charge computed for the molecule and setting the range to match the charge. The range can also be adjusted manually by entering values into the **Charge Range** fields.

The remaining checkboxes in the top portion of this dialog have the following meanings:

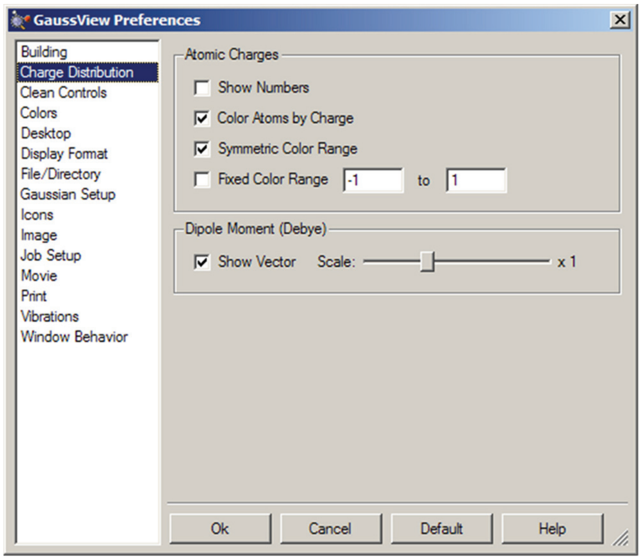
- **Show Numbers**: Place atomic charge values next to each atom.
- **Color Atoms by Charge**: Recolor each atom by atomic charge according to the specifications of the **Color Range** fields and the **Force Symmetric Charge Range** checkbox.
- **Symmetric Color Range**: Forces the positive and negative limits of the charge range to have the same absolute magnitude (regardless of the actual range of the atomic charge values).
- **Fixed Color Range**: Force the charge display to use the default fixed range. This range is set to -1.0 to 1.0 by default, and it can be modified in the **Charge Distribution Preferences**.

The **Dipole Moment** area of the dialog controls whether a vector representing the dipole moment is included in the display. When the vector is displayed, you can specify the scaling factor for the vector's length (the default is about 1.0) as well as its origin.

The buttons at the bottom of the **Display Charge Distribution** dialog control whether the display persists after the dialog is closed. Clicking **Close** will cause the atomic charges display to be retained, while clicking **Cancel** will return the View window to its normal state.

## Charge Distribution Preferences

Defaults for the items in the **Display Atomic Charges** dialog can be set with the **Charge Distribution Preferences** panel (see Figure 85).


GaussView Preferences
Building
Charge Distribution
Clean Controls
Colors
Desktop
Display Format
File/Directory
Gaussian Setup
Icons
Image
Job Setup
Movie
Print
Vibrations
Window Behavior
Ok
Cancel
Default
Help

Atomic Charges

☐ Show Numbers

☑ Color Atoms by Charge

☑ Symmetric Color Range

☐ Fixed Color Range -1 to 1

Dipole Moment (Debye)

☑ Show Vector Scale: x 1

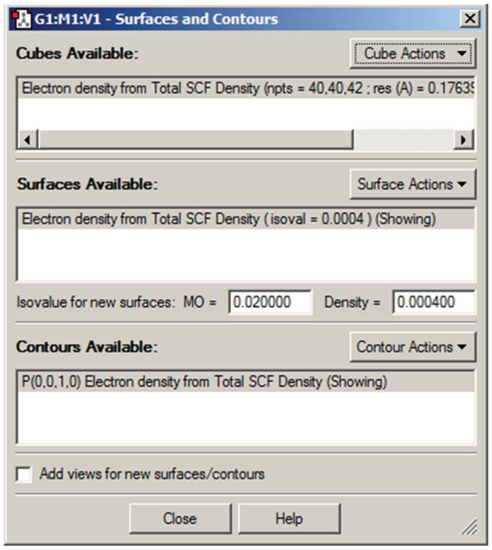
Figure 85. Charge Distribution Preferences

*This preference panel specifies how atomic charge results are visualized, using the same options as in the Charge Distribution dialog.*

## Displaying Surfaces and Contours

The **Results=>Surfaces/Contours** menu item opens the GaussView **Surfaces and Contours** dialog (see Figure 86). It allows you to display various chemical data in three dimensions. The surface data may be generated from a Gaussian checkpoint file or be read in from a cube file. Note that there are two steps involved in actually displaying a surface:

- Obtaining a cube by generating it or reading it in.
- Generating the actual surface for display.


G1:M1:V1 - Surfaces and Contours
Cube Actions
Surface Actions
Contour Actions
Close
Help

Cubes Available:

Electron density from Total SCF Density (npts = 40,40,42 ; res (A) = 0.1763

Surfaces Available:

Electron density from Total SCF Density ( isoval = 0.0004 ) (Showing)

Isovalue for new surfaces: MO = 0.020000 Density = 0.000400

Contours Available:

P(0,0,1,0) Electron density from Total SCF Density (Showing)

☐ Add views for new surfaces/contours

Figure 86. The Surfaces and Contours Dialog

*This dialog allows you to select cubes for display as surfaces and/or contours and also to manipulate currently displayed surfaces and contours.*

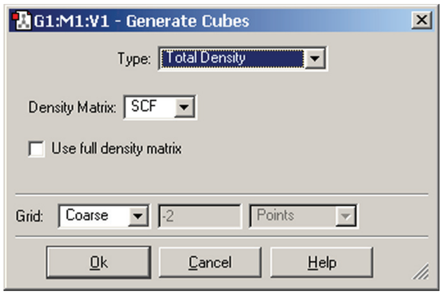
## Generating and Manipulating Cubes

The following items in the **Surfaces and Contours** dialog relate to cubes:

- **Cubes Available**: Shows data that is currently available for display by GaussView. These items appear after cubes are produced using the **New Cube** option and after an existing cube file is loaded.
- **Cube Actions**: Allows you to generate a new cube (**New Cube**), load a cube from an external file (**Load Cube**), save the current cube to an external file (**Save Cube**), and remove the current item from the **Cubes Available** list (**Remove Cube**).

The **New Cube** selection on the **Cube Action** button's menu brings up the dialog in Figure 87. It is used to generate new cubes from the electron density and other data in the checkpoint file. GaussView automatically invokes the CubeGen utility.

The **Type** popup selects the molecular property for which to generate a cube. For most selections, additional fields will appear to further specify the desired data. For example, in Figure 87, the density matrix to use when generating the electrostatic potential cube can be selected. Similarly, for molecular orbitals, the specific orbital(s) to generate are indicated via additional fields.



G1:M1:V1 - Generate Cubes

Type: Total Density

Density Matrix: SCF

☐ Use full density matrix

Grid: Coarse -2 Points

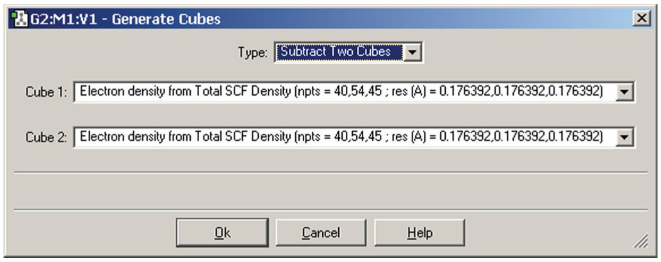
Figure 87. The Generate Cubes Dialog

*This dialog will generate the type of cube specified in the Type field. Here, we are generating a cube of the electrostatic potential computed from the SCF electron density (frozen core by default).*

The **Grid** field is used to specify the density of the cube. Increased density brings increased computational requirements. Generally, the default setting of **Coarse** is adequate for most visualization purposes, **Medium** is adequate for most printing and presentation purposes. The equivalent number of points per "side" is indicated in the second field in this line for each of the **Coarse**, **Medium** and **Fine** selections. Use the **Custom** item to specify a different value.

Clicking the **Ok** button will generate the cube (as a background calculation) and exit the dialog. The new cube will appear in the **Cubes Available** list when the calculation finishes. You can view the job via the **Calculate=>Current Jobs** menu item or the equivalent **Current Jobs** button. *Note*: Cubes generated on the fly in this manner are not saved to disk unless you do so explicitly; otherwise, they will be lost when GaussView terminates.

There are several items in the **Type** popup that allow you to transform one or more cubes: you can scale and square cubes and add or subtract two cubes. For example, if you wanted to display a difference density, you can load in the two cube files (e.g., the densities computed in the gas phase and in solution). Once they are loaded, you can create a new cube (via **Cube Actions=>New Cube**) and then select **Subtract Two Cubes** from the **Type** menu.



G2:M1:V1 - Generate Cubes

Type: Subtract Two Cubes

Cube 1: Electron density from Total SCF Density (npts = 40,54,45 ; res (A) = 0.176392,0.176392,0.176392)

Cube 2: Electron density from Total SCF Density (npts = 40,54,45 ; res (A) = 0.176392,0.176392,0.176392)

Figure 88. Creating a Cube as the Difference of Two Densities

*This dialog creates a new cube that is the difference between corresponding values in the two source cubes.*

## Displaying Surfaces

The following items in the **Surfaces and Contours** dialog relate to surfaces:

- **Surfaces Available**: Displays a list of generated surfaces.
- **Isodensity for new surfaces**: Specifies the isodensity value used for generating new surfaces.
- **Add views for new surfaces**: If checked, a new View window is opened to display the new surface. Otherwise, the surface is displayed in the current View window.
- **Surface Actions**: This button brings up a menu of surface-related actions. Use items here to actually generate the surface in a View window. Note that, once generated, surfaces are tied to their original View window.

The **Surface Actions** menu includes these items:

- **New Surface**: Create a new surface for the selected cube, using the current settings of the related fields in the dialog (i.e., isodensity value and add new view).
- **New Mapped Surface**: Create a new property-mapped surface (see below).
- **Show Surface**: Make this surface visible in its View window.
- **Hide Surface**: Hide this surface in its View window, but retain it for possible later redisplay.
- **Remove Surface**: Discard this surface, removing it from its View window and from the **Surfaces Available** list.

Figure 89 shows some example surfaces.

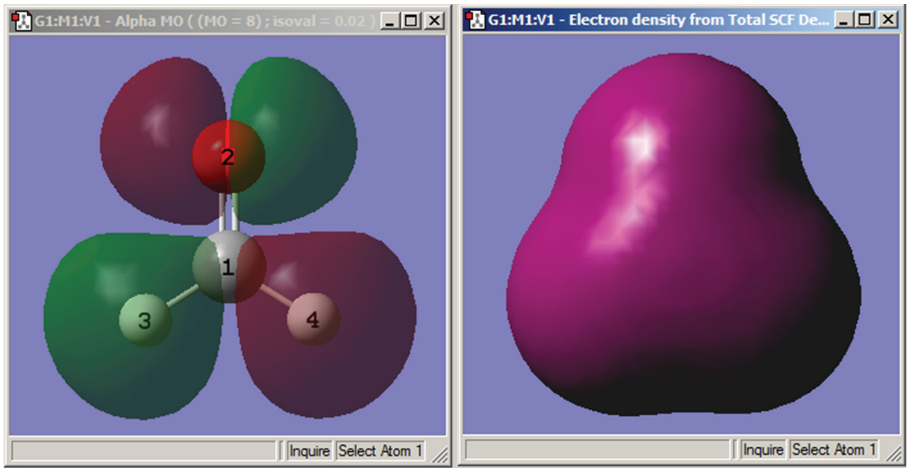

G1:M1:V1 - Alpha MO ( (MO = 8) ; isoval = 0.02 )
2
1
3
4
Inquire
Select Atom 1
G1:M1:V1 - Electron density from Total SCF De...
Inquire
Select Atom 1

**Figure 89.** Example GaussView Surfaces

*These windows display the HOMO molecular orbital surface (left, displayed in transparent mode) and an electron density surface (right, displayed in solid mode). Both are for formaldehyde.*

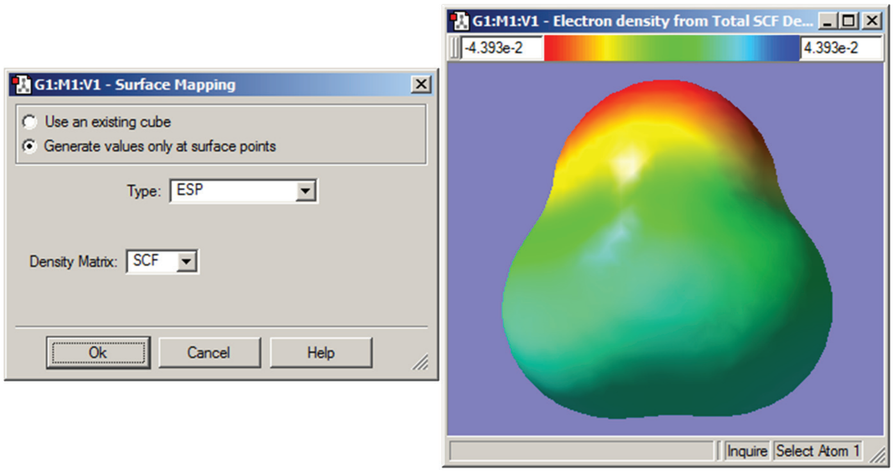
Note that surfaces cannot be saved as data (only cubes can). Rather, they must be recomputed when they are desired. Images of surfaces can also be saved as image files for use in other contexts.

## Mapped Surfaces

GaussView also allows you to map the values of one property on an isosurface of a different property. This is accomplished by selecting the **New Mapped Surface** item from the **Surface Actions** button's menu. This will bring up the dialog illustrated in Figure 90.

The fields in this dialog have the following purposes:

- **Use an existing cube**: Use one of the current cubes as the colorization data. Select the desired surface from the list that is present when this item is selected.


G1:M1:V1 - Surface Mapping
Ok
Cancel
Help
G1:M1:V1 - Electron density from Total SCF De...
-4.393e-2
4.393e-2
Inquire
Select Atom 1

○ Use an existing cube
● Generate values only at surface points

Type: ESP

Density Matrix: SCF

**Figure 90.** Creating a Mapped Surface

*This dialog allows you to create a surface in which the coloring is determined by the values of a second property. The window on the right shows an electron density surface painted according to the value of the electrostatic potential for formaldehyde.*

- **Generate values only at surface points**: Generate the colorization data on the fly at each surface point. This is generally a faster choice (available with Gaussian 03 and later). Specify the desired surface for colorization data in the popup menu and other fields.

View windows display mapped surfaces and include a color mapping toolbar at the top (as in the window on the right in Figure 90). The colors used in rendering a mapped surface are based on a uniform scaling between minimum and maximum values, as specified in the text boxes to the left and right of the spectrum (respectively). Changing the values in these boxes will change the color scale and correspondingly change the coloring on the mapped surface. Like other toolbars, this color mapping toolbar can be moved around the edges by simply clicking and holding on the grip bar and dragging around the window.

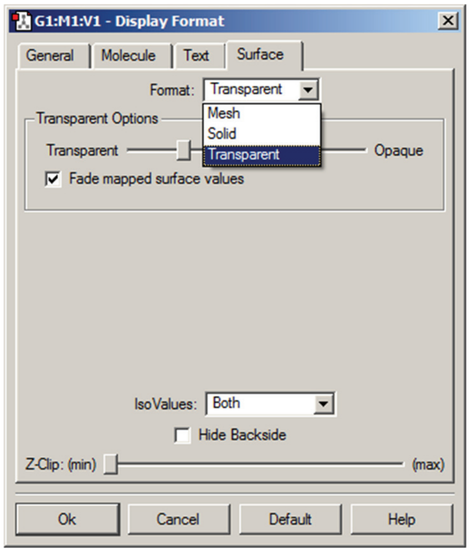
## Customizing Surface Displays

Surfaces may be displayed in solid, transparent and wire mesh forms. The surface display may be modified using the **Display Format** dialog's **Surface** panel (accessed via the **View=>Display Format** menu item and the equivalent **Display Format** button on the toolbar). The dialog format for a transparent surface is displayed in Figure 91.

The **Z-Clip** slider is present in the dialog for all three surface types. It may be used to remove the frontmost portions of the image to allow views into the interior of the molecular display.

The **IsoValues** popup controls whether the positive values, negative values or both (the default) are displayed. The **Hide backside** checkbox controls whether the back side of surfaces are displayed. Checking it results in increased transparency for transparent surfaces. Try turning it on and off with the **Format** set to **Mesh** to see exactly what is being hidden or revealed.

Defaults for surface properties can also be set via the **Display Format Preferences**' **Surface** panel, which contains the same controls as in Figure 91.


G1:M1:V1 - Display Format
General
Molecule
Text
Surface
Mesh
Solid
Transparent
Transparent Options
Transparent
Opaque
Z-Clip: (min)
(max)
Ok
Cancel
Default
Help

Format: Transparent

☑ Fade mapped surface values

IsoValues: Both

☐ Hide Backside

**Figure 91.** Customizing a Surface Display

*This dialog allows you to modify the display of surfaces. Here, we are setting the properties of a transparent surface. The Transparent Options slider varies the opacity of the transparent surface. The Fade mapped surface value checkbox causes the values in the midrange of the spectrum to become transparent (i.e., those close to zero).*

## Displaying Contours

Contours are two dimension projections of cube data into a plane. They also use the cubes generated in the **Surfaces and Contours** dialog (see Figure 86). The items on the **Contour Actions** menu work analogously to those on the **Surface Actions** menu: you can use them to create a new contour (**New Contour**), to display or hide a contour (**Show Contour** and **Hide Contour**) and to remove a contour (**Remove Contour**). Figure 92 illustrates an example contour display.

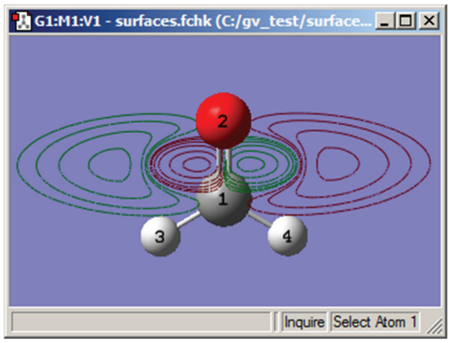

G1:M1:V1 - surfaces.fchk (C:/gv_test/surface...
2
1
3
4
Inquire
Select Atom 1

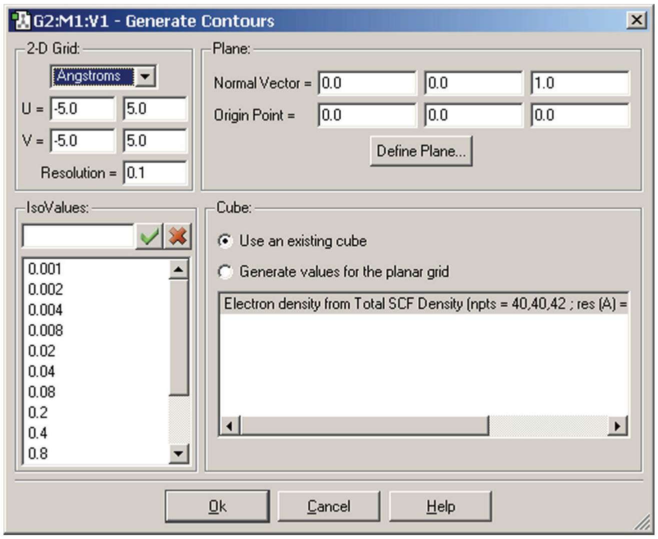
**Figure 92.** Example Contour Plot

*This contour projects the HOMO into a plane perpendicular to the C=O bond.*

Figure 93 illustrates the dialog that results from selecting **Contour Actions=>New Contour**. It contains four subareas:

- **2-D Grid**: Specifies characteristics of the grid used to compute the contour points.You specify the units for the values in this area with the popup menu. The **U** and **V** fields specify the minimum and maximum values in the two grid directions, and the **Resolution** field specifies the distance between grid points.
- **Plane**: Specifies the plane in which the contour will be drawn. This item is discussed below.
- **Cube**: Selects the source of the contour data: either an existing cube (select it from the list) or values generated explicitly for the planar grid. The former is illustrated in Figure 93; the latter is similar to the analogous feature for mapped surfaces (see Figure 87).

- **IsoValues**: Specifies the series of isovalues at which the contour will be computed. You can add or remove items from this list as desired.



G2:M1:V1 - Generate Contours

2-D Grid: Angstroms

U = -5.0 5.0

V = -5.0 5.0

Resolution = 0.1

Plane:

Normal Vector = 0.0 0.0 1.0

Origin Point = 0.0 0.0 0.0

IsoValues:

0.001
0.002
0.004
0.008
0.02
0.04
0.08
0.2
0.4
0.8

Cube:

● Use an existing cube

○ Generate values for the planar grid

Electron density from Total SCF Density (npts = 40,40,42 ; res (A) =

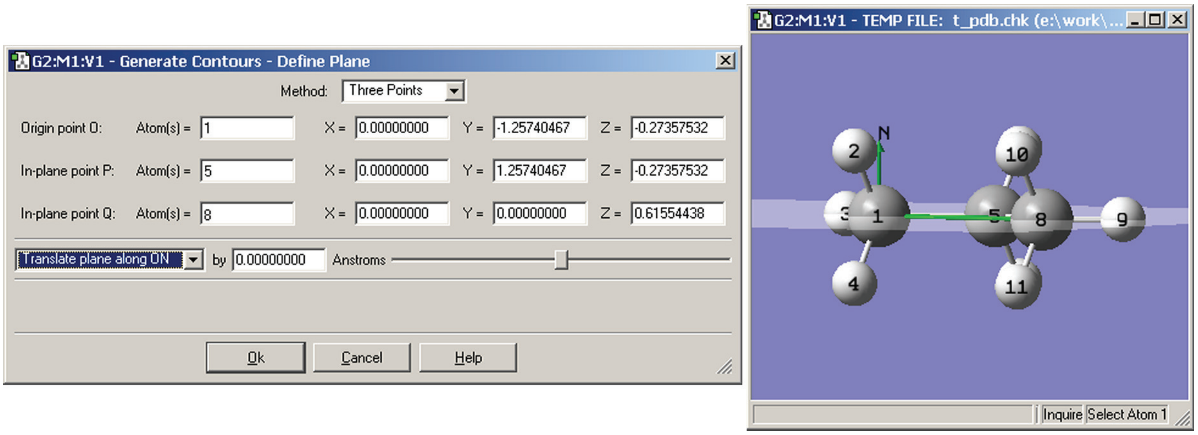
Figure 93. The Generate Contours Dialog

*This dialog will generate a contour from an existing cube created or loaded previously via the Cube Actions menu in the Surfaces and Contours dialog.*

### Defining the Contour Plane

By default, the contour plane is defined as the view's XY plane. The plane can be defined in the **Contour** dialog's **Plane** area. It is defined as the plane perpendicular to the vector defined by the specified **Normal** and **Origin** points in the dialog. The default origin point is (0,0,0) and the default point defining the normal vector is (0,0,1).

More complex plane definitions can be specified by clicking on the **Define Plane** button, which brings up the dialog in Figure 94. There are two methods for defining the plane: **Normal Vector** (as described above) and **Three Points** (illustrated in the figure). In the latter method, you define the origin and two other points to define the contour plane (traditionally referred to as O, P and Q). The easiest way to define the points is to specify atoms for them, but you can also enter lists of atoms (the average of their coordinates will then be used) or completely arbitrary Cartesian coordinates.



G2:M1:V1 - Generate Contours - Define Plane

Method: Three Points

Origin point O: Atom(s) = 1 X = 0.00000000 Y = -1.25740467 Z = -0.27357532

In-plane point P: Atom(s) = 5 X = 0.00000000 Y = 1.25740467 Z = -0.27357532

In-plane point Q: Atom(s) = 8 X = 0.00000000 Y = 0.00000000 Z = 0.61554438

Translate plane along ON by 0.00000000 Anstroms

G2:M1:V1 - TEMP FILE: t_pdb.chk (e:\work\...

Inquire Select Atom 1

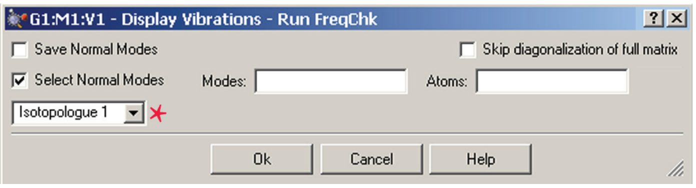
Figure 94. Specifying the Desired Contour Plane

*In this example we are defining the contour plane as the one containing the carbon atoms, using the 3 points definition method. The green lines in the View window indicate the normal vector (labeled N) at the origin (O) and the line OQ. The OP line is not visible in this view as it mirrors the C-C bond between atoms 1 and 5.*

Once the contour plane is defined, you can move it further using the popup and other controls in the bottom part of the dialog. The plane can be translated or rotated about the various defined axes.

## Displaying Vibrational Modes and IR/Raman Spectra

The **Results=>Vibrations** menu item is used to access various spectral results from frequency calculations. It allows calculated vibrational data to be displayed as dynamic screen motions, based on information from a frequency calculation. When you have retrieved results from a Gaussian checkpoint file or formatted checkpoint file, this menu item initially displays the **Run FreqChk** dialog, illustrated in Figure 95. If you have opened a Gaussian log file, you are taken directly to the **Display Vibrations** dialog (see Figure 96).



G1:M1:V1 - Display Vibrations - Run FreqChk

☐ Save Normal Modes

☐ Skip diagonalization of full matrix

☑ Select Normal Modes

Modes:

Atoms:

Isotopologue 1

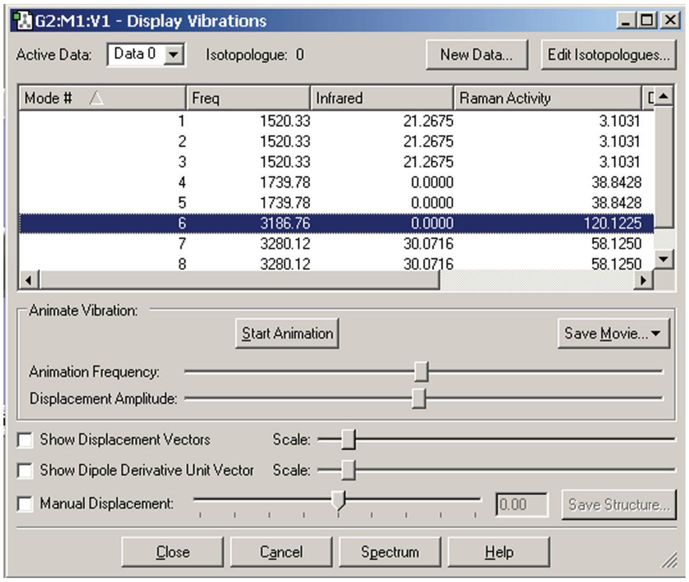
Figure 95. Running FreqChk to Perform Vibrational Analysis

*This dialog is used to run the freqchk utility included with Gaussian. This utility performs vibrational analysis for the isotopologue specified in the popup menu in the left portion of the dialog (the menu is marked with a star); here the analysis will be performed for the second isotopologue. Once complete, the modes and spectra are available for visualization via the Display Vibrations dialog.*

The **Save Normal Modes** and **Select Normal Modes** items are relevant only with Gaussian 09. They correspond to the **Freq=SaveNormalModes** and **Freq=SelectNormalModes** options, respectively (and to the equivalent FreqChk options). The former saves computed normal modes back to the checkpoint file, and the latter limits the vibrational analysis to the listed modes (**Modes**) and modes involving the listed atoms/atom types (**Atoms**). The **Skip diagonalization of full matrix** corresponds to **Freq=NoDiagFull**.

Once you exit the **Run FreqChk** dialog, the utility will run, and the **Display Vibrations** window will open. It is illustrated in Figure 96 as it appears after FreqChk completes.

The items in the top row of the dialog allow you to select which isotopologue's data is displayed (the **Active Data** popup menu). The **New Data** button opens the **Run FreqChk** dialog, and the **Edit Isotopologues** button opens the **Atom List Editor**. See Figure 99 for an example of displaying vibrational data for multiple isotopologues.



G2:M1:V1 - Display Vibrations

Active Data: Data 0

Isotopologue: 0

| Mode # | Freq | Infrared | Raman Activity |
|---|---|---|---|
| 1 | 1520.33 | 21.2675 | 3.1031 |
| 2 | 1520.33 | 21.2675 | 3.1031 |
| 3 | 1520.33 | 21.2675 | 3.1031 |
| 4 | 1739.78 | 0.0000 | 38.8428 |
| 5 | 1739.78 | 0.0000 | 38.8428 |
| 6 | 3186.76 | 0.0000 | 120.1225 |
| 7 | 3280.12 | 30.0716 | 58.1250 |
| 8 | 3280.12 | 30.0716 | 58.1250 |

Animate Vibration:

☐ Show Displacement Vectors

☐ Show Dipole Derivative Unit Vector

☐ Manual Displacement: 0.00

Figure 96. The Display Vibrations Window

*This dialog displays a table of all computed spectra from frequency calculations. In this case, we see the vibrational frequencies, infrared intensities, Raman intensities and VCD rotational strengths. The window's Spectrum button is used to access graphical representations of the predicted spectra.*

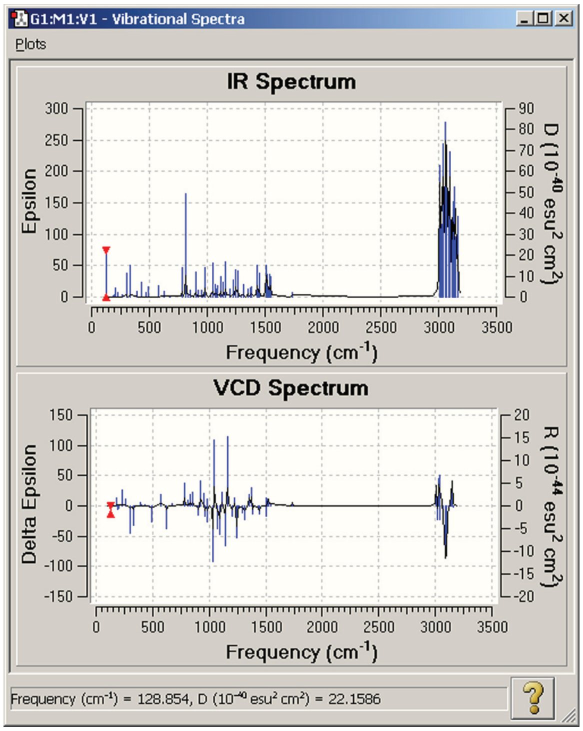
The **Display Vibrations** dialog shows which vibration is currently selected for dynamic display. You can start this display by selecting the **Start Animation** button, and halt it by clicking on the **Stop Animation** button. The molecule will begin a cyclical displacement showing the motions corresponding to the vibration selected. The two slide bars below the **Start/Stop Animation** button adjust the speed and magnitude of the motion. Default values for these settings may be specified in the **Vibrations Preferences** panel (as well as for the displacement and dipole derivative unit vector which are discussed below).

The animation can also be saved as a movie and/or as individual frames using the **Save Movie** button (see the discussion of saving movies earlier in this manual for more information).

You can select other modes by selecting the desired mode in the scrolling list. You can select a new mode without halting the previous one. You can also rotate and move the vibrating molecule, using the normal mouse buttons.

## Displaying the Spectrum

The **Spectrum** button presents Gaussian's estimate of the spectrum in line format. Note that the intensity values are relative to the highest value in the present set, and bear no precise relationship to experimental band intensities. Example spectra are illustrated in Figure 97. Clicking on the various peaks within the spectra is another method for selecting which vibration mode is currently animated.


G1:M1:V1 - Vibrational Spectra
Plots
IR Spectrum
Epsilon
300
250
200
150
100
50
0
D ($10^{-40}$ esu$^2$ cm$^2$)
90
80
70
60
50
40
30
20
10
0
0
500
1000
1500
2000
2500
3000
3500
Frequency (cm$^{-1}$)
VCD Spectrum
Delta Epsilon
150
100
50
0
-50
-100
-150
R ($10^{-44}$ esu$^2$ cm$^2$)
20
15
10
5
0
-5
-10
-15
-20
0
500
1000
1500
2000
2500
3000
3500
Frequency (cm$^{-1}$)

Frequency (cm$^{-1}$) = 128.854, D ($10^{-40}$ esu$^2$ cm$^2$) = 22.1586

Figure 97. GaussView Spectra Displays

*These plots display the IR and VCD spectra graphically. The available spectra depend on the Gaussian calculation that was run.*

## Vector-Based Displays

The two vector-related checkboxes in the bottom section of the Display Vibrations dialog have the following meanings (see Figure 87 for examples):

- **Show Displacement Vectors**: Display the motion associated with the vibration as a displacement vector in the View window.
- **Show Dipole Derivative Unit Vector**: Display the dipole derivative unit vector as a vector in the View window.

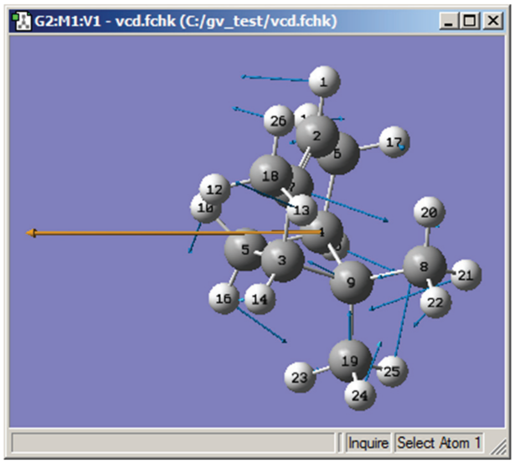


**Figure 98.** Displaying the Displacement Vector and Dipole Derivative Unit Vector
*The various displacement vectors are displayed in blue, and the dipole derivative unit vector is the orange arrow on the left.*

### Using Manual Displacement Display Mode

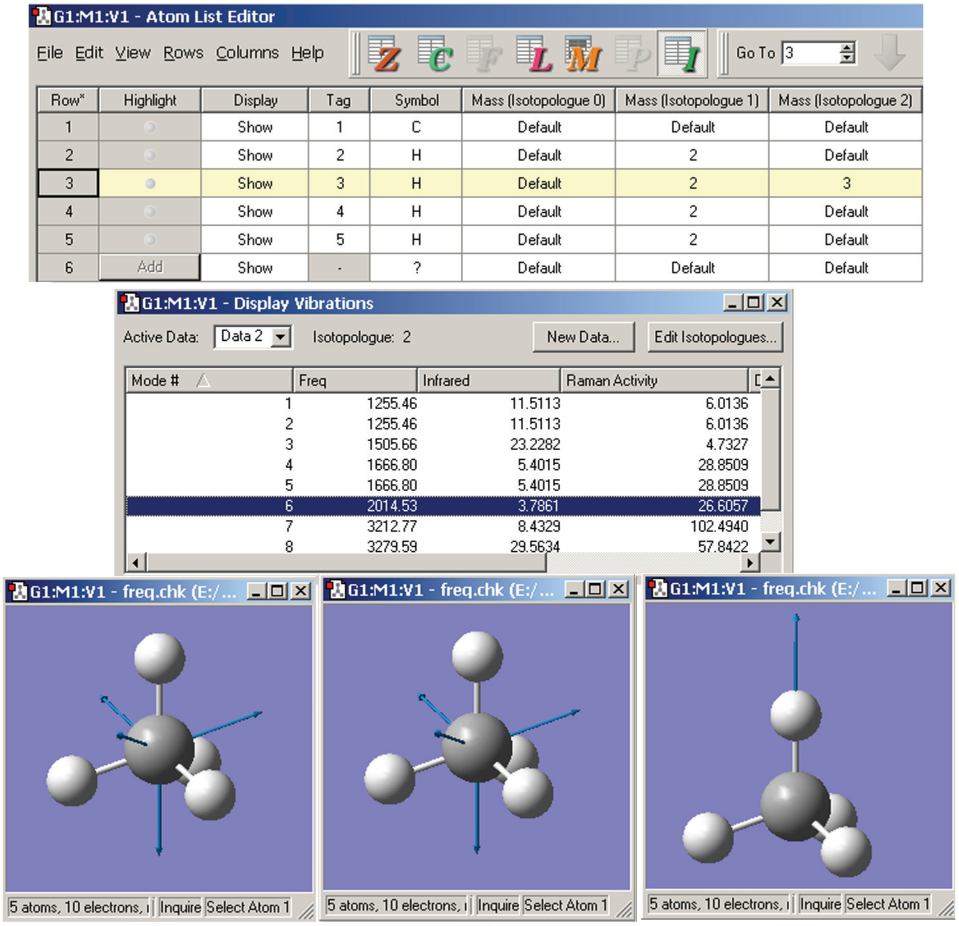
The **Manual Displacement** box allows you to set the displacement as desired. When it is checked, animation of the vibration will be turned off. When checked, the slider, number box, and **Save Structure** button become active. In this mode, changing the slider or the corresponding number box will cause the molecule to be statically displaced along the currently active normal mode. The center value of the slider, or zero in the text box, corresponds to no displacement. Moving the slider to the right or entering a positive value in the text box will displace the atoms along the currently active normal mode. Moving to the left or entering a negative value will displace the atoms in the direction opposite of the currently active normal mode. The range of values allowed in the text box ranges from -1 to +1. Clicking on **Save Structure** will cause a new molecule window to appear with a geometry exactly corresponding to the displaced structure.

The primary use of this tool is to help eliminate spurious negative eigenvalues. hen one is searching for a transition state, it is not uncommon to end up with a structure containing two (or more) negative eigenvalues instead. These spurious negative eigenvalues are generally small but must be eliminated to isolate the true transition state. For these cases, select the normal mode corresponding to the spurious negative eigenvalue, and then select **Manual Displacement**. Adjust the slider to the right (or enter a positive number in the text box), and then select **Save Structure** to create a new molecule with the displaced geometry, which you can then reoptimize. If a positive displacement fails to eliminate the spurious negative eigenvalue, follow the same procedure with a displacement in the negative direction. You can also try varying the magnitude of the displacement.

A second purpose of manual displacement is to generate pictures of a molecule in the midst of a vibration. Thus, it can be used to effectively freeze the animation of the vibration at a specific point.

## Comparing Spectra for Isotopologues

GaussView makes it easy to compare spectra for different isotopologues of the same structure. To do so, you first define the desired isotopes for each isotopologue using the **Atom List Editor**. Then you generate vibrational data sets for each one. Once completed, you can use the **Display Vibrations** dialog to examine the spectra and normal modes.


G1:M1:V1 - Atom List Editor
File Edit View Rows Columns Help
Go To 3
G1:M1:V1 - Display Vibrations
New Data...
Edit Isotopologues...
G1:M1:V1 - freq.chk (E:/...
5 atoms, 10 electrons, i
Inquire
Select Atom 1

| Row* | Highlight | Display | Tag | Symbol | Mass (Isotopologue 0) | Mass (Isotopologue 1) | Mass (Isotopologue 2) |
|---|---|---|---|---|---|---|---|
| 1 | | Show | 1 | C | Default | Default | Default |
| 2 | | Show | 2 | H | Default | 2 | Default |
| 3 | | Show | 3 | H | Default | 2 | 3 |
| 4 | | Show | 4 | H | Default | 2 | Default |
| 5 | | Show | 5 | H | Default | 2 | Default |
| 6 | Add | Show | - | ? | Default | Default | Default |

Active Data: Data 2 Isotopologue: 2

| Mode # | Freq | Infrared | Raman Activity |
|---|---|---|---|
| 1 | 1255.46 | 11.5113 | 6.0136 |
| 2 | 1255.46 | 11.5113 | 6.0136 |
| 3 | 1505.66 | 23.2282 | 4.7327 |
| 4 | 1666.80 | 5.4015 | 28.8509 |
| 5 | 1666.80 | 5.4015 | 28.8509 |
| 6 | 2014.53 | 3.7861 | 26.6057 |
| 7 | 3212.77 | 8.4329 | 102.4940 |
| 8 | 3279.59 | 29.5634 | 57.8422 |

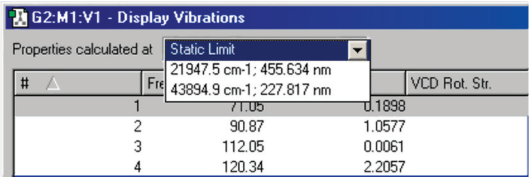
3187 2254 2015

**Figure 99.** Setting Up Isotopologues and Comparing Normal Modes

*In the Atom List Editor (top), we have defined three isotopologues for this simple molecule: one with the standard isotopes, one with deuterium replacing each hydrogen, and a third with tritium replacing a single hydrogen. The normal mode corresponding to the sixth frequency shifts location for each isotopologue (compare the values beneath each View window). The motion for the first two isotopologues is similar, but the mode for the tritium form has the motion confined to that atom.*

## Frequency-Dependent Calculation Results

Gaussian frequency calculations can specify values for the electromagnetic field perturbation at which to compute vibration properties. GaussView allows you to specify the desired incident light frequency for such frequency-dependent calculations by adding a popup menu to the top of the **Display Vibrations** window, as illustrated in Figure 100.


G2:M1:V1 - Display Vibrations
Static Limit
21947.5 cm-1; 455.634 nm
43894.9 cm-1; 227.817 nm

Properties calculated at Static Limit

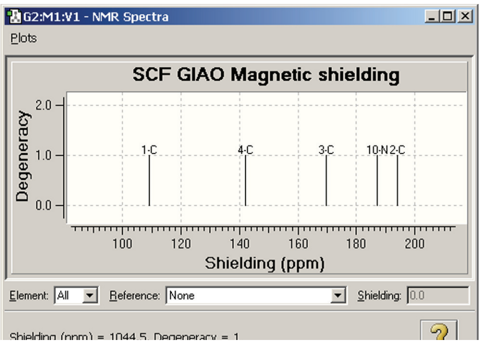
| # | Fre | VCD Rot. Str. |
|---|---|---|
| 1 | 71.05 | 0.1898 |
| 2 | 90.87 | 1.0577 |
| 3 | 112.05 | 0.0061 |
| 4 | 120.34 | 2.2057 |

**Figure 100.** Specifying a Specific Frequency

*GaussView adds this menu at the top of the Display Vibrations window for frequency-dependent calculation results. The Static Limit selection corresponds to a standard frequency calculation.*

## Displaying NMR Spectra

The **Results=>NMR** menu item displays the spectrum from an NMR calculation. An example spectrum is shown in Figure 101.


G2:M1:V1 - NMR Spectra
Plots
SCF GIAO Magnetic shielding
Degeneracy
2.0
1.0
0.0
1-C
4-C
3-C
10-N
2-C
100
120
140
160
180
200
Shielding (ppm)

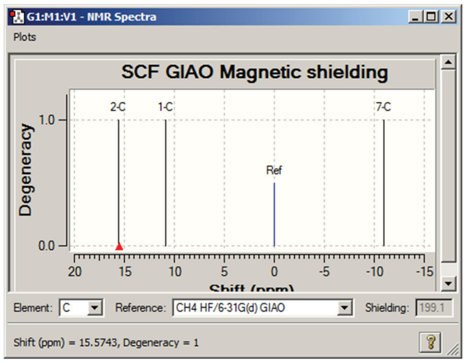
Element: All
Reference: None
Shielding: 0.0

Shielding (ppm) = 1044.5, Degeneracy = 1

**Figure 101.** NMR Spectrum Display

*This is the default NMR display format. It displays all computed peaks. Clicking on a peak with the cursor displays the shielding value and degeneracy in the lower left corner of the window (e.g., peak 2-C above)*

The fields at the bottom of the **NMR Spectra** window allow you to view the same data as relative values with respect to TMS or other standards (see Figure 102). To use this feature, first select the desired element in the leftmost popup menu, and then select one of the available standard calculation results from the **Reference** field. The peaks will then reflect relative values with respect to the selected reference.


G1:M1:V1 - NMR Spectra
Plots
SCF GIAO Magnetic shielding
Degeneracy
1.0
0.0
2-C
1-C
Ref
7-C
20
15
10
5
0
-5
-10
-15
Shift (ppm)

Element: C
Reference: CH4 HF/6-31G(d) GIAO
Shielding: 199.1

Shift (ppm) = 15.5743, Degeneracy = 1

**Figure 102.** Displaying NMR Chemical Shifts

*Clicking on a peak in this display mode shows the numeric chemical shift with respect to the specified standard in the lower left corner of the window. The corresponding shielding value is displayed in the Shielding field.*

## Displaying UV-Visible Spectra

The **Results=>UV-VIS** menu item displays the spectra computed by an excited states calculation. An example spectrum is displayed in Figure 103.

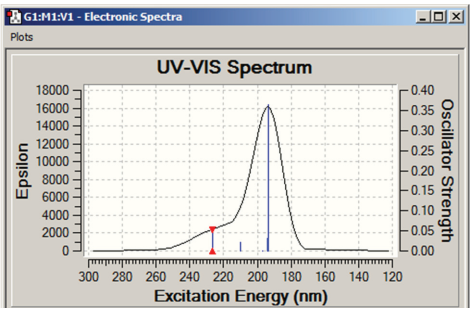
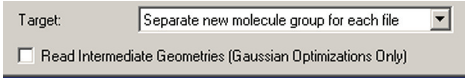

G1:M1:V1 - Electronic Spectra
Plots
UV-VIS Spectrum
Epsilon
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
Oscillator Strength
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
300
280
260
240
220
200
180
160
140
120
Excitation Energy (nm)

**Figure 103.** Example UV-Visible Spectrum Display

*Additional spectra may be viewed for excited states calculations, including ECD for chiral molecules.*

# Viewing Optimization Results and Other Structure Sequences

When you open a results file containing such results from optimizations, potential energy surface scans, IRC calculations or ADMP or BOMD trajectory calculations, you will need to check the **Read intermediate geometries (optimization only)** checkbox in the **Open File** dialog in order to retrieve all of the geometries that are present (see Figure 104). When you do so, each geometry that is present becomes a separate model within a new molecule group (by default). Note that this checkbox applies to all of these job types, despite being labeled **optimization only**.



Target: Separate new molecule group for each file

☐ Read Intermediate Geometries (Gaussian Optimizations Only)

**Figure 104.** Retrieving Intermediate Results from Optimizations and Similar Jobs
*The setting in the Target field above is the recommended one for opening files containing multiple structures. Don't forget to check the Read intermediate geometries checkbox, or only the final structure will be retrieved.*

You can animate the various structures using the buttons in the View window's toolbar when the View window is set to single model mode. Animation begins by pressing the green circle button in the toolbar. The animation can then be stopped via the red X icon which replaces it. The animation speed is controlled by the **Animation Delay** setting in the **General** panel of the **Display** preferences.

The remaining items on the **Results** menu (**Scan**, **IRC**, **Trajectory**, **Optimization**) all allow you to view plots of energy and other results from calculations that produce multiple structures among their results. Figure 105 illustrates the displays for a geometry optimization.

The specific plots that appear vary by job type:

- Optimizations: **Total Energy** and **RMS Gradient**.
- Potential Energy Surface Scans: **Scan of Total Energy**.
- IRC Reaction Path: **Total Energy Along IRC** and **RMS Gradient Along IRC**.
- Trajectory (ADMP or BOMD): **Nuclear Kinetic Energy**, **Electronic Kinetic Energy**, **Potential Energy**, **Total Energy**, **Total Angular Momentum**, **Conservation of Alpha Electrons**, **Average Alpha Idempotency**, **RMS Alpha Idempotency**, **Conservation of Beta Electrons**, **Average Beta Idempotency**, and **RMS Beta Idempotency** (the latter three apply only to open shell calculations).

You can click on the various points in the plot, and the corresponding structure will appear in the View window.

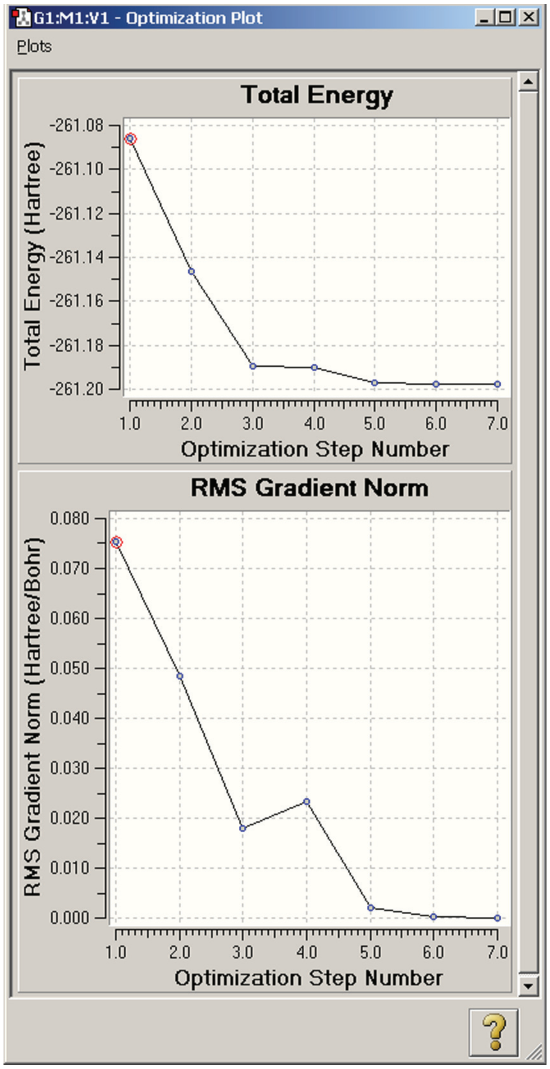
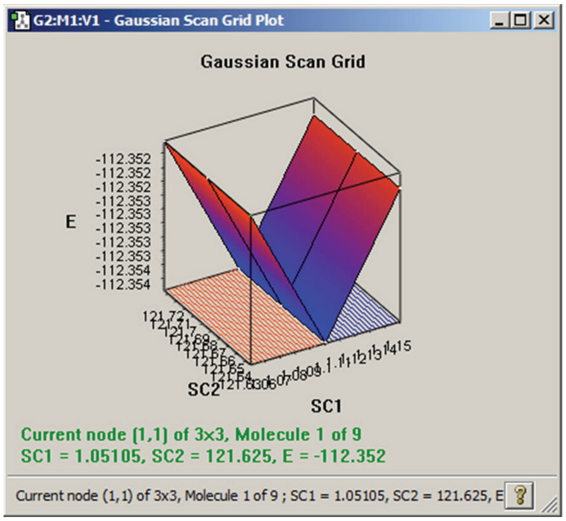

G1:M1:V1 - Optimization Plot
Plots
Total Energy
Total Energy (Hartree)
-261.08
-261.10
-261.12
-261.14
-261.16
-261.18
-261.20
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Optimization Step Number
RMS Gradient Norm
RMS Gradient Norm (Hartree/Bohr)
0.080
0.070
0.060
0.050
0.040
0.030
0.020
0.010
0.000
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Optimization Step Number
?

**Figure 105.** Plots from a Geometry Optimization
*These plots display the total energy and root-mean-square gradient for each optimization point.*

## Viewing 3D Plots of 2-Variable Scan Calculations

Gaussian **Scan** calculations over two variables are plotted by GaussView as three dimensional surfaces. An example appears in Figure 106. You can click on the various points in this plot as for 2D plots.


G2:M1:V1 - Gaussian Scan Grid Plot
Gaussian Scan Grid
E
-112.352
-112.352
-112.352
-112.353
-112.353
-112.353
-112.353
-112.353
-112.354
-112.354
SC2
SC1

Current node (1,1) of 3x3, Molecule 1 of 9
SC1 = 1.05105, SC2 = 121.625, E = -112.352

Current node (1,1) of 3x3, Molecule 1 of 9 ; SC1 = 1.05105, SC2 = 121.625, E

Figure 106. Results Plot for a PES Scan over 2 Variables

*Only scan calculations over exactly two variables will produce plots like this one. Note that this plot can be rotated and zoomed using the standard mouse actions.*

## Plotting Additional Properties

You can create additional plots of various properties for these job types. This is done by selecting the **Plots=>Plot Molecular Property** menu item in the plot window. This results in the dialog in Figure 107.

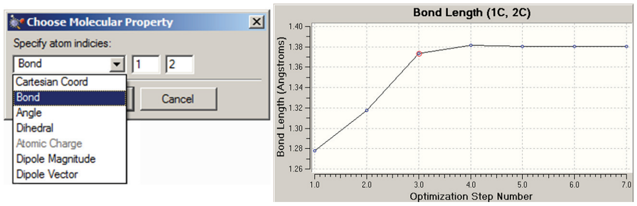

Choose Molecular Property
Specify atom indicies:
Bond
1
2
Cartesian Coord
Bond
Angle
Dihedral
Atomic Charge
Dipole Magnitude
Dipole Vector
Cancel
Bond Length (1C, 2C)
Bond Length (Angstroms)
1.40
1.38
1.36
1.34
1.32
1.30
1.28
1.26
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Optimization Step Number

Figure 107. Creating An Additional Plot

*In this example, we are adding a plot displaying the C-C bond distance for atoms 1 and 2 over the course of the geometry optimization. The dialog at the left displays the various items that may be plotted.*

The items available for plotting vary by the job type. Once generated, the new plot appears below the standard ones in the plots window.

## Correcting Plot Discontinuities

When data is read in for a multi-geometry plot, the values along the X-axis should form a single continuous ascending set. In some occasions, a user may include molecules from two or more different files within the same molecule group. This is sometimes useful for comparison purposes or to extend the output from a previous run. When this occurs, the X-axis values will no longer form a single continuous ascending set, resulting in a jagged appearance in the resulting plot. When this situation is detected, an informational message is displayed.

The **Plots=>Fix Discontinuity** menu item may be used to correct such plots. When this feature is used, the words "(Modified)" are added to the title of the plot to remind the user that the data in the plot has been modified and so should be viewed with caution.

## Manipulating and Customizing Plots and Spectra

All plots and spectra can be manipulated for viewing in a variety of ways:

- Scrolling and resizing: Typically multiple plots/spectra are available in the same dialog and will not all be viewable at the same time. In that case, the dialog window can be resized to see more of them at the same time or the user can use the scroll bar to scroll down to see the desired plot. If several plots are visible then resizing the window expands/shrinks the X-axis while the plot height stays constant. In other words, only the height of the viewing area changes.

  When only one plot is visible—i.e., the dialog only contains one plot or the other plots have been hidden (see below)—then resizing the dialog expands/shrinks the plot along both axes. To focus on one or two plots, hide the other plots using the **Plots** menu.

- Hiding individual plots/spectra: The upper section of the **Plots** menu, illustrated in Figure 108, contains a list of all currently available items. You can hide or reveal individual items within the list by removing/restoring the checkmark before the item name (respectively). The **Show All Plots** item will always reveal (check) all items. The **Hide Other Plots** on the context menu (see below) will hide all but the currently displayed item.

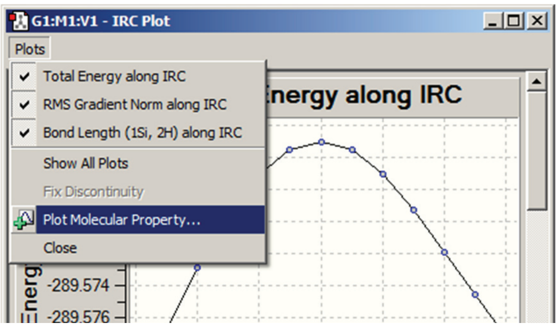
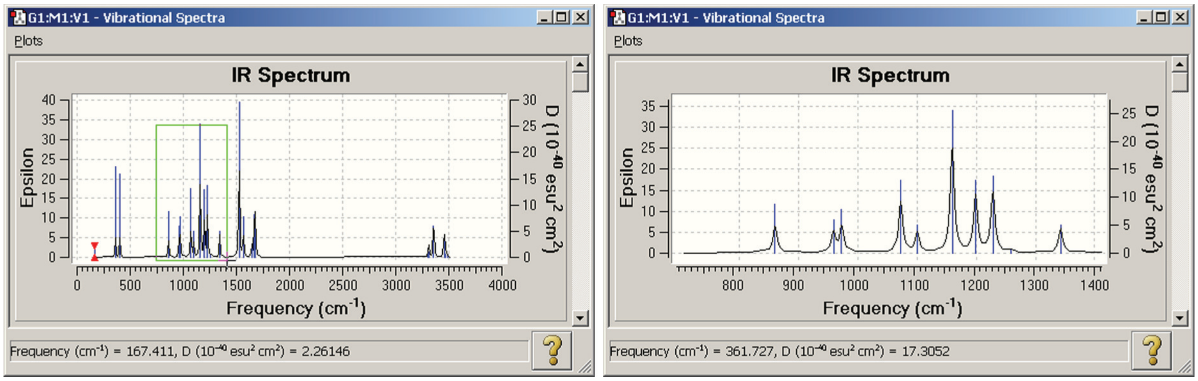

G1:M1:V1 - IRC Plot
Plots
✓ Total Energy along IRC
✓ RMS Gradient Norm along IRC
✓ Bond Length (1Si, 2H) along IRC
Show All Plots
Fix Discontinuity
Plot Molecular Property...
Close
nergy along IRC
Energ
-289.574
-289.576

Figure 108. The Plots Menu

*This menu is found in all plot and spectra windows. This particular example comes from the plots window displayed for an IRC calculation. Currently, all available plots are visible.*

- Zooming and unzooming: All of the plots and spectra support zooming. This feature is very handy for resolving fine details. To zoom in, click and hold the left mouse button to select one corner of the zoom field. While holding the mouse button down, move the mouse to opposite corner of the desired zoom area. The zoom area will be marked with a green rectangle (see Figure 109). Release the mouse button, and the selected area will be zoomed to fill the full area. You can keep zooming in as much as you want. To unzoom (i.e., restore the original view), use the plot context menu's **Zoom Out** item.


G1:M1:V1 - Vibrational Spectra
Plots
IR Spectrum
Epsilon
0
5
10
15
20
25
30
35
40
D (10$^{-40}$ esu$^2$ cm$^2$)
0
5
10
15
20
25
30
0
500
1000
1500
2000
2500
3000
3500
4000
Frequency (cm$^{-1}$)
G1:M1:V1 - Vibrational Spectra
Plots
IR Spectrum
Epsilon
0
5
10
15
20
25
30
35
D (10$^{-40}$ esu$^2$ cm$^2$)
0
5
10
15
20
25
800
900
1000
1100
1200
1300
1400
Frequency (cm$^{-1}$)
?

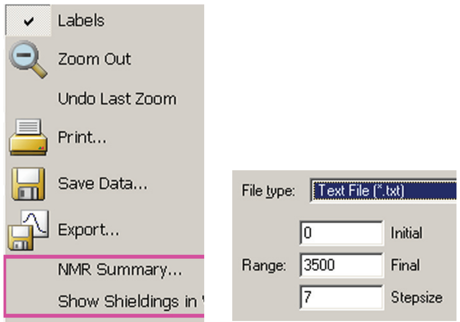
Frequency (cm$^{-1}$) = 167.411, D (10$^{-40}$ esu$^2$ cm$^2$) = 2.26146

Frequency (cm$^{-1}$) = 361.727, D (10$^{-40}$ esu$^2$ cm$^2$) = 17.3052

Figure 109. Zooming In on a Spectrum

*The spectrum on the left is the one initially displayed by GaussView. Here, we are zooming in on the area in green. The resulting view is displayed on the right.*

- Context menu: Right clicking in the plot or spectrum, including the gray section containing the title and axis labels, will bring up a context menu for that specific plot/spectrum. The options in the menu generally apply only to the current item. The context menu is illustrated in Figure 110. The items have the following meanings:
  - **Show All Plots** and **Hide Other Plots** reveal all items and hide all but the current item, respectively.
  - **Zoom Out** restores the original plot appearance, undoing all zooming. **Undo Last Zoom** reverses only the most recent zoom operation.
  - **Print** prints the current plot or spectrum.
  - **Save Data** allows you to save the plot or spectrum data to a text file. For the latter, fields labeled **Range** are added to the standard operating system Save dialog to allow you to select a subset of the data for inclusion.
  - **Export** allows you to save the plot or spectrum as a graphics file.
  - **Properties** allows you to customize many aspects of the plot. It is discussed in detail in the next subsection of this manual.



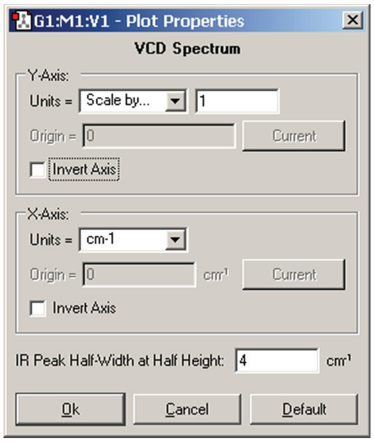
File type: Text File (*.txt)

Range: 0 Initial
3500 Final
7 Stepsize

**Figure 110.** The Plot/Spectrum Context Menu and Save Data Range Fields
*The menu on the left appears when you right click within a plot or spectrum. Only applicable items will be included and active. The fields on the right are added to the standard Save dialog when you select Save Data for a spectrum.*

## Customizing Plots and Spectra

Figure 111 appears when you select the **Properties** item from the context menu for a plot or spectrum.



Y-Axis:
Units = Scale by... 1
Origin = 0
☐ Invert Axis

X-Axis:
Units = cm-1
Origin = 0 cm-1
☐ Invert Axis

IR Peak Half-Width at Half Height: 4 cm-1

**Figure 111.** Customizing a Plot/Spectrum
*This dialog may be used to customize many aspects of a plot or spectrum. Not all controls are active for all item types. Note that the field at the bottom of the dialog varies according to the spectrum type (here, we are working on a vibrational spectrum).*

The various controls in the dialog have the following effects:

- **Units**: Specifies the units for the corresponding axis. Coordinates can also be scaled by selecting the **Scale by** from the popup menu and entering value into the text box (see the Y-axis in Figure 99).
- **Origin**: Specifies the value for the origin for the corresponding axis.
- **Current** buttons: Causes the coordinate of the currently selected point to be used as the origin for the corresponding axis.
- **Invert Axis**: Invert the plot vertically (Y-axis) or horizontally (X-axis).
- **Default** button: Restore all items to their default values.

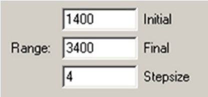
Other fields that may appear in the dialog include the following:

- **IR Peak Half-Width at Half Height**: Specifies the width of peaks in vibration spectra. Making the value larger makes the peaks wider.
- **UV-Vis Peak Half-Width at Half Height**: Specifies the width of peaks for UV-Visible spectra. Making the value larger makes the peaks wider.
- **NMR Degeneracy Tolerance**: The threshold for determining when peaks of spectra in the NMR Spectra dialog can be grouped. Making the value larger may cause more peaks to be grouped together as degenerate. Setting the value to zero means that no peaks will be treated as degenerate.

## Saving Plot Data

The context menu for plots and spectra contains the **Save Data** item. This may be used to save the numeric data corresponding to a plot/spectrum to an external file. Here is an example of the data saved from an0 IR spectrum:

```
# IR Spectrum
# X-Axis:  Frequency (cm-1)
# Y-Axis:  Epsilon
#            X                     Y                DY/DX
      1400.0000000000        0.2434072675        0.0040413306
      1404.0000000000        0.2604146278        0.0044720368
      1408.0000000000        0.2792680154        0.0049661578
      ...
```



Range: 1400 Initial
3400 Final
4 Stepsize

You can specify the range of data and step size between points for this kind of data via the additional fields that GaussView adds to the standard Save dialog (illustrated to the right of the data above).

Data from plots of geometry optimizations, IRC calculations and the like can be saved in the same way. Here is some example data from an IRC calculation:

```
# Total Energy along IRC
# X-Axis:  Intrinsic Reaction Coordinate
# Y-Axis:  Total Energy (Hartree)
#             X                     Y
        -0.5999778220     -289.5812430000
        -0.4999857200     -289.5768190000
        -0.3999923250     -289.5728940000
        ...
```

For NMR spectra, an additional summary file may also be written, using the **NMR Summary** item on the spectrum's context menu. Here is an example:

```
# Summary of NMR spectra ( SCF GIAO Magnetic shielding)
# Degenerate peaks are condensed together (Degeneracy Tolerance 0.05)
#
#     Shielding (ppm)     Degeneracy Elem    Atoms
        26.6182000000         1.0000  H       1
        27.7949000000         2.0000  H       5,6
        76.9883000000         1.0000  C       2
        93.9401000000         1.0000  C       3
       106.1777000000         1.0000  C       4
```

# Index

## A

active space
    *See* CASSCF
ADMP 92
amino acids 17
animations 11, 63
    individual frames 64
    multiple structures 6
    normal modes 88
    optimizations 92
    saving 63
    speed 6
antiferromagnetic coupling 74
Atom Group Editor 27
    defining fragments 74
    frozen atoms 73
    group types/uses 28
    NMR spin-spin coupling 74
    selecting normal modes 74
atomic charges 79
Atom List Editor 6, 26, 30, 31, 34
    isotopologues 87
    link atoms in 73
    sorting rows in 12
    sublist filters 33
atoms 31
Atom Selection Editor 28
atoms types for MM 11, 30, 72
axes, displaying in views 9, 51

## B

ball and stick display 54
basis sets 68
Biological Fragments palette 17
BOMD 92
bond angles
    modifying 20
    viewing 18
bond lengths
    modifying 19
    viewing 18
bonds
    adding/removing 19
    coloring of 56
    rebonding 24
    specifying type 19
Builder palette 3, 15, 18, 26
    context menu 17
    icon sizes in 13
building molecules
    *See* molecules: building
Building Preferences 48

## C

calculation summary 79
capturing images 62
Cartesian coordinates 30
CASSCF
    Gaussian input 73
    manipulating MOs for 41
centroid position
    placing fragment at 17
Charge Distribution Preferences 80
charges
    defining for MM 32
    displaying atomic 79
    molecular 27
    per-fragment 27, 74
checkpoint file 68
    quick launch and 76
chemical shifts 91
Clean Controls Preferences 22, 23
clean function 22
    performance 24
clipboard 7, 8, 31
colorization of surfaces 84
colors
    atomic charges 80
    atom labels 55
    for each element 56
    image background 63
    surfaces 56
    vectors 56
    view background 52
Colors Preferences 56
Connection Editor 35, 72
context menus 6
    Builder palette 17
    plots & spectra 95
    schemes 75
    toolbar 3
    view 5
contours 85
    plane definitions 86
control panel 2
coordination patterns for elements 15
counterpoise calculations 74
CPK molecule display 54
crowded atoms 32
Crystal Editor 42
cubes 81
    contours and 85
    generating 82
    operations with 82
Current Fragment display 2
    fragment placement options 48
custom command line 78
custom fragment library 29
Custom Fragments palette 29
cutting and pasting 7, 8, 58

## D

dangling half bonds 11
data, saving
    *See* exporting numerical data
default directory 64
degenerate orbitals 41
deleting
    atoms 22
    molecules 58
    selected atoms 8
Desktop Preferences (Windows) 65
difference density 82
dihedral angles
    modifying 20
    viewing 18
dipole derivative unit vector 88
dipole moment 80
displacement vector 88
Display Atomic Charges dialog 79
Display Charge Distribution dialog 80
Display Format dialog 6, 51, 52, 55
    surfaces and 84
Display Format Preferences 6, 51-52
    periodic systems 47
    surface-related settings 84
Display Vibrations dialog 87, 88, 89
distance algorithm 24
DNA bases 17
drag and drop (Windows) 58
dummy atoms 9, 18

## E

electron density 82
Element Fragments palette 15
exiting GaussView 7
exporting numerical data
    molecular structures 31
    MO-related 42
    NMR summary 97
    plots & spectra 96
extensions (Windows) 65

## F

file associations (Windows) 65
File/Directory Preferences 64

- filters
  - in Atom List Editor 33
- fog 53
- fonts 55
- fractional coordinates 30, 44, 45
- fragment guess calculations 74
- Fragment Placement Options 11, 48
- fragments
  - Atom Group Editor and 27, 74
  - centroid position 17
  - charge & spin 27
  - defining custom 29
  - Gaussian input and 71
  - handling when bonds/angles change 19–21
  - limiting mouse action to 6
  - palette 16
- frequency calculations
  - *See* vibrational analysis, IR spectra
- frozen atoms 73
- functional groups
  - *See* fragments

## G

- Gaussian Calculation Setup dialog 66
  - additional input 72
  - antiferromagnetic coupling calculations 75
  - basis sets 68
  - CASSCF and 73
  - defaults for 75
  - fragments and 71
  - frequency calculations 74
  - initial guess 70
  - job types 67
  - Link 0 commands 68
  - methods 67
  - MOs and 70
  - NMR spin-spin coupling 74
  - ONIOM calculations 73
  - PBC calculations 71
  - schemes 75
  - solvation calculations 71
  - title section 68
- Gaussian Setup Preferences 75
- GAUSS_SCRDIR 64
- graphics files
  - supported types 62
- gray scale images 61
- grids 82

## H

- help 10
  - tips 10, 14
  - tutorials 1, 42
- highlighting 32
  - appearance of 26
- hot atom, defined 48
- hybridizations 15
- hydrogens
  - adding 11, 21
  - adding to imported structs. 32, 60
  - deleting 31
  - showing/hiding 9, 51

## I

- icons
  - Atom List Editor 11
  - manipulating items in lists 12
  - selection 26
  - specifying sizes for 13
  - table of 7
  - thumbtacks 11
- Icons Preferences 13
- images
  - background color for 63
  - enlarging 62, 63
  - plot & spectra 64
  - printing 61
  - resolution of 62
  - saving 62
  - saving MO diagram 42
- importing
  - *See* molecules: importing
- incident light frequency 90
- initial guess 70
- input files
  - constructing 66–71
  - editing 67
- inquire mode 18
- intensity values 88
- interatomic distance
  - *See* bond lengths
- internal variables 78
- IRC calculations 92
- IR spectra 87, 88
- isodensity 83
- isotopes 12, 30
  - comparing results for 90
  - defining 34

## J

- Job Manager dialog 76
- jobs
  - *See also* submitting jobs, Gaussian Calculation Setup dialog
  - launch options 77
  - scripts for 77
  - terminating 76
  - viewing status 76
- Job Setup Preferences 76
- job types 67

## K

- keywords, Gaussian
  - additional 67
- K-points 71

## L

- labels, viewing 51
- layers
  - *See* ONIOM: layers
- Layer Selection Tool 37
- libraries (of fragments) 29
- Link 0 commands 68
- link atoms 72
- log files
  - *See also* output
  - editing 9
  - opening associated 79
- lone pairs 60

## M

- manual displacement display mode 89
- marquee selection 26
- menus 7
  - table of items 7
- methods 67
  - default 67
- Miller index 47
- mirror invert (symmetry) 22
- MM Charges dialog 32
- model groups 4
  - *See also* molecule groups
- modifier keys 7
- molecular orbitals 39–40
  - Gaussian input and 70
  - modifying occupancy 41
  - reordering 42
  - saving image of diagram 42
  - surfaces 83
  - visualizing 40
- molecule groups 4
  - adding & removing views 58
  - animating 6, 11
  - creating 58
  - importing multiple structures to 59
  - view color coding by 5
- molecule positioning toolbar 9, 52
- molecules
  - aligning atoms in multiple 35
  - building 15, 19–21
  - cleaning 22
  - deleting 58
  - display options 51
  - exporting structural data 31
  - importing 59
  - imposing symmetry 24
  - modifying structure 19
  - opening 59
  - rebonding 24
  - reverting to read-in structure 60
  - saving 61
  - viewing structural info 18
- MOs dialog 39

mouse, operations with 6
  in Connection Editor 36
  in spectra 94
  limiting to one fragment 6
  plots 92
movies
  *See* animations
multiview mode 4
  animating 6
MultiView Options dialog 4, 5

## N

NBO analysis 71
negative eigenvalues 89
Newman projection 20
NMR
  exporting summary data 97
  results 91
  spin-spin coupling 74
normal modes
  animating 88
  selecting 74
nucleosides 17

## O

occupancy diagram 41
ONIOM
  calculation setup 73
  display options for 53
  Gaussian input for 72
  layers 30, 37
  link atoms 72
  MM atom types & charges 32
  rigid blocks 73
open valences 11
optimizations
  animating results 92
  frozen atoms 73
  results from 92
  to transition structure 72
Options for Opening Files dialog 60
output 76
  streaming 9

## P

palettes
  making sticky 17
partial charge density 79
PBC 42–48, 72
  *See also* unit cells
  building a unit cell 42
  Gaussian input for 71
PDB files
  adding hydrogens to 32, 60
  opening options for 60
  secondary structures from 34
  viewing info from 11, 30, 35
PDB Residue Editor 26, 34
PDB Secondary Structure Editor 26, 34
periodic systems
  *See* PBC
periodic table 15
  changing colors 56
plots
  3D from scans 93
  adding properties to 93
  context menu 95
  customizing 95
  exporting numeric data 96
  fixing discontinuities 93
  IRC reaction paths 92
  mouse operations in 92
  optimizations 92
  saving images of 64
  scans 92
  trajectories 92
Point Group Symmetry dialog 24
preferences 12
  Building 48
  Charge Distribution 80
  Clean Controls 22, 23
  Colors 56
  Desktop (Windows) 65
  Display Format 6, 51, 52, 84
  File/Directory 64
  Gaussian Setup 75
  Icons 13
  Job Setup 76
  Print 61
  restoring defaults 13
  Vibrations 88
  Window Behavior 13
printing
  images 61
  molecular structural data 31
Print Preferences 61

## Q

QST2/QST3 optimizations 72
quick launch 75

## R

Raman spectra 87
reaction paths
  *See* IRC
read intermediate geometries 59, 92
rebonding 24
  in unit cells 44
redo 7
Redundant Coordinate Editor 36, 37
redundant internal coordinates 73
reorienting molecules 51
residues
  defining ONIOM layers with 37, 38
  editor for 34
  retaining in Gaussian input 69
  selecting by 29
  sorting structure by 31
  viewing 30
resolution, image 62
results 79–97
  excited states calculations 91
  from gradient calculations 92
  summary 79
R-Group Fragments palette 16
rigid blocks 73
Ring Fragments palette 16
rotating 6
rubberband selection
  *See* marquee selection
Run FreqChk dialog 87

## S

saving
  *See* molecules: saving, images: saving, exporting numerical data
scans 92
  3D plots of 93
schemes 75
scratch files 64
SCRF 71
scripts 77
  internal variables for 78
selecting atoms 6, 11, 26
  appearance of 26
  customizing behavior for 29
  dialog for 28
  in Editor dialogs 26
  keystrokes for 26
serial numbers 9
SmartSlides 19
smoothing, display 52
solvation 71
space group symmetry 43
  constraining 44
spectra
  comparing by isotopologue 89
  context menu 95
  customizing 95
  exporting numeric data 96
  IR/Raman 87, 88
  NMR 91
  saving images of 64
  UV-Visible 91
  zooming 94
spin multiplicity
  per-fragment 27, 74
spin-spin coupling, NMR 74
spotlighting 52
status bars
  info in 18, 25
stereochemistry
  labeling atoms by 9
STQN optimizations 72
structures
  *See* molecules
Sublist Filters dialog 33
submitting jobs 66, 75
  quick launch 75

summary, calculation 79
surfaces 81
    display options 85
    generating 83
    mapped 83
    specifying colors for 56
Surfaces and Contours dialog 81, 85
symmetry
    imposing 24
    in periodic systems 43
    inverting about an atom 22
    setting tolerance for 25
synchronizing views 57

T

thumbtack icons 11, 17
tips 10, 14
title section 68
toolbars 2
    context menu 3
    separated 3
torsion angles
    *See* dihedral angles
trajectory plots 9, 92
transition structure optimizations
    aligning atoms for 35
    Gaussian input 72
translating structures 6
transparent surfaces 84
tube molecule display 54, 55
tutorials 1
    PBC 42

U

undo 7
unit cells
    building 43
    in the Atom List Editor 32
    rebonding 44
    reducing 47
    symmetry in 43
    vertices of 46
utilities 76

V

valences 21
    adding 21
    deleting 11
    *See also* hydrogens, open valences
van der Waals radii-based display 54
VCD spectra 88
vectors 56
    dipole derivative 88
    dipole moment 80
    displacement 88
vibrational analysis 87
    *See also* normal modes
    frequency-dependent 90
Vibrations Preferences 88
views 3
    adding 8, 57
    centering 51
    context menu 5
    creating 58
    display options 9, 51
    display quality 52
    saving images from 62
    selection keystrokes in 26
    synchronizing 4
    within the MOs dialog 39

W

Window Behavior Preferences 13
windows
    *See also* views
    changing background color 52
    customizing behavior of 13
    hiding and restoring 57
    selection keystrokes 26
    single view vs. multiview 4
    symmetry display in 25
    synchronizing 4, 57
    title bar color coding 5
    viewing angle/distance values in 18
    working with 10
wireframe molecule display 54
work directory 64

Z

Z-matrix 30, 31
zooming 6