

QUANTA 2006

Generating and Displaying Molecules

MAY 2006

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Contents

Preface: Preface	1
Who should read this book	1
What this book contains	1
How to use the QUANTA introductory documentation set	2
Documentation set roadmap	2
Related documentation	3
Restarting QUANTA	4
Conventions	4
1. Sketching 2D Molecules	5
Starting ChemNote	5
Understanding the ChemNote window	6
Menu bar	6
Palette	10
Message line	11
Creating a 2D sketch	11
Rings	11
Bonds	12
Changing atoms within a structure	15
Carbon substitution	15
Hydrogen atoms	17
Customizing bonds	19
Saving ChemNote structures	20
Returning to Molecular Modeling	23
Importing a .mol file into Molecular Modeling	24
Using templates	26
The Template window	27
Title bar	27
Menu bar	27
Buttons	27
Building a template-based structure	28
Summary	36
2. Editing 3D Structures	39
Creating a base structure	39
Editing bonds and fragments	41
Customizing the Fragment Table	47
Altering atoms	47
Minimizing a structure	52
Saving a structure	53
Saving and exiting with multiple structures	56
Other editing options	60
Summary	63
3. Calculating and Minimizing Energy	65
Understanding basic CHARMM operations	65
The CHARMM energy functions	65
CHARMM theory	66
CHARMM calculations	66

QUANTA interaction with CHARMM	67
Generating a potential energy value	70
Performing a minimization	71
Performing repeated minimizations	74
Saving or rejecting calculation results.	75
The Merck Molecular Force Field	76
Summary	77
References	78
4. Building with Sequence Builder	79
Understanding the Sequence Builder window	80
Starting Sequence Builder	82
Building a sequence	84
Creating a peptide	87
Minimizing a peptide	90
Creating a cyclic peptide.	91
Summary	94
5. Using Other Build Applications	97
Using Crystal Modeling	97
Defining and incorporating symmetry information.	98
Using the Crystal Modeling palette.	99
Calculating CHARMM energy using images	99
Modifying the asymmetric unit	102
Using protein applications	107
Using X-ray applications	108
Using NMR Structure Determination.	108
Summary	109
6. Using Graphical Objects	111
Generating ribbons	112
Generating a grid contour mesh.	113
3D vector displays	114
QUANTA plot files	115
Color scale	115
Managing objects	116
Solvent surfaces	117
Displaying probe interaction results	122
Displaying molecule interaction results	125
Calculating electrostatic interactions only	130
Managing maps.	133
Generating an electrostatic potential energy surface	134
Calculating and displaying an electrostatic potential grid map	135
Calculating and displaying an electrostatic potential dot surface	139
Calculating and displaying an isoenergy 2D contour plots 141	141
Generating an electrostatic field	143
Generating and displaying hydrogen bonds	144
Applying settings to other structures	150
Summary	152
References	152
7. Generating Visual Representations	155
Rendering solid models	155
Manipulating solid models.	157

Using the Solid Model window	159
Sample procedure — Generating a solid model	160
Generating cartoons of proteins and nucleic acids.	163
Generating solid surfaces.	166
Generating raytrace van der Waals models	168
Generating display-only raster models	169
Plots for hardcopy output	169
MolScript plots.	174
Summary	176
8. Importing and Exporting Files	179
Importing PDB files	180
PDB import/export preferences	180
PDB files containing multiple models	180
Importing Protein Data Bank files	181
Importing multiple PDB files	181
Cleaning imported structures	181
Splitting tools	182
Cleaning tools.	183
Exporting an MSF	184
9. Using External Applications	187
Accessing external programs from QUANTA	187
Specifying a host	187
Performing a calculation on a remote host	188
Using CINDO	188
Using MOPAC	193
Executing a single-energy AM1 calculation.	197
Comparing MOPAC data	201
Using UHBD.	202
Summary	202
CINDO	202
MOPAC	203
UHBD	203
References	204

Who should read this book

QUANTA Generating and Displaying Molecules is designed primarily for first-time users. You can read it to understand how to create, import, and edit molecules within QUANTA.

If you are an experienced user, read this book to review information on functionality and procedures for executing building and editing tasks of QUANTA or to update yourself on changes since previous versions of QUANTA.

What this book contains

This book contains information for building, importing, editing, and manipulating 2D and 3D molecules. Performing these functions, using a variety of sketchers and builders, is described in Chapters 1, 2, 4, and 5.

Chapter 3 describes CHARMM, the calculation engine of QUANTA, and the processes for performing molecular energy and minimization calculations using CHARMM. Chapter 10 describes how to connect to other external applications for additional calculations and functions.

Chapters 6 and 7 describe ways to use graphical objects and various molecular representations to display and study structures.

Chapter 8 describes importing and exporting files to and from non-QUANTA programs. It includes the steps you take to make sure that any imported molecule is accurately represented within QUANTA.

Chapter 9 describes connecting to specific external calculation applications.

Information provided in progressive chapters is based on the assumption that you are familiar with basic software operations and with material in previous chapters.

Since this book is designed primarily for new users, neither the descriptions nor the tutorial exercises comprehensively document all aspects of using QUANTA.

The book is written assuming that you are familiar with:

- Basic UNIX commands and file and directory structures.
- Windowing software on your workstation.
- The difference between a shell window and a console window on your workstation.
- How your workstation mouse works.

Assumptions also are made that you have a home directory where you can create subdirectories and a licensed copy of QUANTA installed on your workstation.

How to use the QUANTA introductory documentation set

This book is part of a documentation set that introduces QUANTA. The set consists of:

- *Basic Operations*
- *Generating and Displaying Molecules*
- *Simulation, Search, and Analysis*

Although each book is self-contained, information within the set flows in a logical sequence. You must be familiar with basic operations to successfully complete building and editing tasks. Molecule preparation in the building and editing phase must precede simulation and analysis.

Within each book, exercises are step-by-step procedures that may be linked across chapters. Datafiles may be modified or reused by several exercises.

Because of the sequential nature of the documentation set and of the exercises in each book, you will get the most coherent and complete view of the software if you go through the books in sequential order.

Documentation set roadmap

The table below lists key topics and where to find information about them in the introductory set of QUANTA books. Book names are abbreviated:

- Ops— *Basic Operations*
- Gen— *Generating and Displaying*

- SA — *Simulation, Search, and Analysis*

For information about	Look at
Understanding program layout and design	Ops Chapter 1
Using operating principles and procedures	Ops Chapter 2
Manipulating molecules and displays	Ops Chapter 2, Gen Chapters 6 And 7
Building structures	Gen Chapters 1,2,4, and 5
Editing structures	Gen Chapters 1, 2 And 8, SSA Chapter 4
Applying constraints for CHARMM calculations	SSA Chapter 2
Importing and exporting files	Gen Chapter 8
Executing calculations using CHARMM or external programs	Gen Chapters 2, 3, 4, 6, And 9, SSA Chapter 1
Handling data - visual displays, tables, graphs	Ops Chapter 2, Gen Chapters 6 and 7 SSA Chapters 8 and 9
Performing experimental simulations	Gen Chapter 3, SSA Chapters 1, 3-5, 7
Analyzing data	SSA Chapter 6

Related documentation

In addition to the introductory books, other books in the QUANTA documentation set include:

- *QUANTA Installation and Administration*
- *CHARMM Principles*
- *CHARMM Dictionary I and II*

Other QUANTA-related documentation is included with specific software application packages. This documentation includes:

- *Protein User's Reference*
- *Protein Homology Modeling Tutorial*
- *X-Ray Structure Analysis User's Guide*
- *NMR Structure Determination User's Guide*
- *MCSS/Hook User's Guide*

Restarting QUANTA

This book assumes you have already run QUANTA. If you have not, refer to *Setting the QUANTA Environment* and *Starting QUANTA* on pages 4–6 in the book *QUANTA Basic Operations*.

For this and subsequent startups, enter the command:

```
> cd ~/subdirectory
```

Then enter the command:

```
> quanta
```

QUANTA opens displaying the structure you worked on most recently in this directory. The Molecule Management table displays the structure's name and status.

Conventions

Typographical conventions used in this book are:

This	Looks like this
Examples of file contents, information in the textport or on the message line	<code>Fixed-width</code>
Menu and palette names and choices	Bold
Place-holders that you replace with another word	<i>Italic</i>

1. Sketching 2D Molecules

This chapter describes ChemNote, the QUANTA application for building 2D molecules. Read this chapter if and when you plan to generate or significantly modify structures to use in QUANTA.

With ChemNote, you can create 2D molecular sketches that can be converted to 3D structures for use in other QUANTA applications. Sketches are created by progressively selecting and positioning various rings, bonds, and atoms, or by selecting and modifying sketches supplied with the application.

In addition to using drawing and editing tools in ChemNote, you can assign and display chemical properties such as partial atomic charges, saturation, chirality, isotopes, and cis/trans and axial/equatorial marks. The application also provides control over the display of carbon and hydrogen symbols within the sketch.

Information about a sketch is saved in a .mol file. ChemNote creates a .pct file that saves the 2D graphical data for continued use within ChemNote. ChemNote also creates a residue topology file (RTF) that is used by CHARMM to generate a principle structure file (PSF). ChemNote automatically names the RTF by capitalizing the first four letters of the .mol filename and adding a .rtf extension.

The ChemNote .mol file automatically converts to a molecular structure file (MSF) when you exit ChemNote and return to the Molecular Modeling application. This conversion also occurs when an existing .mol file is imported into Molecular Modeling.

Note: ChemNote commands cannot be recorded using the **File | Record Session** commands.

Starting ChemNote

ChemNote runs in a separate window that is opened over the startup QUANTA windows. Activity in Molecular Modeling mode is frozen until you return to the Molecular Modeling window.

1. Sketching 2D Molecules

1. Start QUANTA

If you have not already started QUANTA, do so.

If you have been working systematically through the tutorial exercises, the file `newpeptide.msf` is displayed in the viewing area.

2. Start ChemNote

ChemNote is started from QUANTA's menu bar.

To start ChemNote, display the **Applications** menu. Select **Builders**, open the pull-right menu, and select **2D Sketcher**.

The ChemNote window is displayed over the QUANTA windows, which are frozen until you exit ChemNote.

Understanding the ChemNote window

The ChemNote window can be moved, iconified, pushed, and popped in the same manner as all other standard workstation windows. The window has these four distinct areas:

- Menu bar
- Palette
- Viewing area
- Message line

Although some window areas are the same as those of other QUANTA applications, the menu bar and palette are specifically customized for ChemNote.

Menu bar

The menu bar contains five menus, whose functions are summarized in [Table 1](#).

Table 1. ChemNote menu bar

Menu	Description
File	Creates, retrieves, appends, saves, or prints structures. Returns to the Molecular Modeling application.
Edit	Provides editing operations such as copy, cut, and paste. Controls marking functions. Compresses the display of a group of atoms and alternates between compressed and expanded views at will.
Layout	Controls the display and appearance of atoms and their names. Specifies bond attributes.
Properties	Assigns and displays atom properties. Checks atom valence. Specifies structure geometry, typing, and charging. Controls CHARMM parameters and provides a selection of CHARMM conversion options. Offers three methods for defining monomers.
Help information	Provides software copyright and version number

sketching
2D

ChemNote menus are displayed as pull-down or sticky menus. Tables 2 through 6 list the selections on each menu and briefly describe their functions.

Table 2. File menu

Selection	Description
New	Stores the contents of the viewing area in a specified file and clears the viewing area in preparation for creating another file.
Open	Displays a previously stored file in the viewing area.
Append	Adds a previously created file to the file currently displayed in the viewing area.
Template	Displays the template window to incorporate structures or portions of structures into a sketch.
Save	Saves the content of the viewing area in a specified file.
Save as Template	Saves the content of the viewing area as a specified template.
Print	Prints the contents of the viewing area.
Return to Mol. Modeling	Exits ChemNote and returns control to Molecular Modeling.

1. Sketching 2D Molecules

Table 3. Edit menu

Selection	Description
Cut	Deletes marked objects from the viewing area and places them on the ChemNote clipboard.
Copy	Creates an exact duplicate of marked objects in the viewing area and places it on the ChemNote clipboard.
Paste	Inserts the contents of the ChemNote clipboard into the viewing area.
Delete	Deletes marked items.
Mark All Atoms	Marks all of the objects in the viewing area.
Reverse Marks	Marks any objects in the viewing area that are not currently marked and vice versa.
Unmark All	Removes marks from all of the objects in the viewing area.
Create Shortcut	Creates a shortcut from the currently delimited part of a structure.
Compress Shortcut	Reduces the previously defined shortcut group to a place holder.
Expand Shortcut	Regenerates the drawing by replacing the placeholder atom with the original shortcut grouping.
Destroy Shortcut	Removes the association of atoms forming a shortcut group.

Table 4. Layout menu

Selection	Description
Element Name	Displays the atomic symbol for marked atoms.
Atom Name	Displays a user-defined atom name for marked atoms.
Ionic Charge	Displays an integer representation of the charge on an atom.
Partial Charge	Displays an approximation of the charges shared between neighboring atoms.
Display Carbons	Displays the atomic symbol "C" for the marked carbon atoms.
Suppress Carbons	Hides the atomic symbol "C" for the marked carbon atoms.
Display Hydrogens	Displays automatically supplied hydrogen atoms attached to the marked atoms as bonded "H" atomic symbols.
Abbreviate Hydrogens	Displays automatically supplied hydrogen atoms attached to the marked atoms in a condensed notation such as CH ₃ .
Suppress Hydrogens	Hides automatically supplied hydrogen atoms attached to the marked atoms.
Saturate Atoms	Displays marked atoms as saturated.
Unsaturate Atoms	Displays marked atoms as unsaturated.

Table 4. Layout menu

Selection	Description
Thin Bonds	Displays all bonds as thin lines.
Thick Bonds	Displays all bonds as thick lines.
Standard Length	Defines bonds of a fixed length that match the length of the bonds in rings or match a user defined length.
Standard Angles	Defines bond angles to be drawn at 15° increments or to a user-defined value.
Redraw Screen	Redisplays all items in the viewing area

Table 5. Properties menu

Selection	Description
Assign Atom Properties	Assigns properties to individually marked atoms.
Display Atom Properties	Controls the visibility of atomic properties of a marked atom.
Conversion Options	Sets CHARMM conversion options.
Check Valence	Checks that all atoms have the proper valence.
Cis/Trans Marks	Specifies cis/trans orientation for double bonds. This function can be accessed from the palette.
Axial/Equatorial	Sets axial/equatorial bond orientation.
Torsion Angle	Sets torsion angle.
Reset Types	Resets all CHARMM atom types to unknown type.
Reset Charges	Sets all partial charges to zero.
Type Atoms	Assigns CHARMM types to all atoms.
Charge Atoms	Calculates partial charges for all atoms.
Charge Marked Atoms	Calculates partial charges for marked atoms.
Define Monomer	Converts a molecule into a monomeric unit.
Rename Backbone	Renames backbone atoms in monomeric unit.

Table 6. Information menu

Selection	Description
About ChemNote	Provides current program version information.

Palette

The palette contains selections that you use to create and edit a 2D sketch. Use these tools either to perform various operations or to create actual sketch components such as atoms, bonds, and rings. The palette highlights the current selection. Table 7 lists and briefly describes the selections and tools.

In addition to the palette tools, ChemNote provides techniques for manipulating sketches. These include dragging a sketch or portion of a sketch with the right mouse button to reset it in the viewing area, or marking a sketch or portion of a sketch with a rubber band rectangle technique

Table 7. ChemNote palette

Selection	Description
Point	Marks objects for subsequent action. This selection is automatically in effect at the start of a ChemNote session.
Lasso	Encircles irregularly shaped areas in the structure for marking atoms.
Font	Establishes type attributes such as type style and size for displayed atom labels.
Merge Structures	Merges atomic structures.
Move Items	Moves marked atoms and bonds.
Eraser	Erases marked atoms and bonds.
Periodic Table	Displays a dialog box containing the Periodic Table for atom selection.
Atom Symbols	Allows selected atoms to be placed in the viewing area.
Bond Icons	Allows selected bond to be placed in the viewing area.
Ring Icons	Allows selected ring to be placed in the viewing area.
Reflect Y-Axis	Flips marked objects about the y axis.
Reflect X-Axis	Flips marked objects about the x axis.
Rotate	Rotates marked objects.
Scale	Scales marked objects.
Aromatize	Aromatizes or dearomatizes marked rings.
Axial/Equatorial	Defines the marked bond as axial, equatorial, or neither.
Cis/Trans	Defines the marked bond as cis, trans, or neither.
Set Torsion	Allows specification of a dihedral angle for viewing and calculations.

Message line

Help messages are displayed at the bottom of the application window in the message line. Information is provided in dialog boxes displayed in the viewing area. These generally provide options for defining selection criteria.

Creating a 2D sketch

Various rings and bonds are available from the palette to create 2D sketches. Using the mouse, you can add objects to the viewing area by making a selection from the palette, moving the cursor to the viewing area, and anchoring each object. You can move, rotate, or merge anchored objects with other objects.

ChemNote highlights atoms and bonds as the cursor is moved over them. This gives a visual cue to help select objects once they have been placed in the viewing area.

When you use the mouse to select and place various parts of a molecule, click rapidly. Delay in clicking the mouse can yield a different event.

Rings

Rings are defined from the palette by selecting one of nine available icons. ChemNote automatically assigns carbon atoms to each ring as it is drawn, and automatically supplies hydrogen atoms to meet valence requirements. Carbon and aliphatic hydrogen element symbols are not displayed by default. However, both carbon and hydrogen symbols can be displayed. Use the following practice exercise to become familiar with using ring tools.

1. Place a six-membered ring in the viewing area.

Move the cursor over one of the six-membered ring tools. Two graphical representations for each of the five- and six-membered rings are provided as a drawing aid. They have the same 3D conformation.

Click the left mouse button and a ring icon is highlighted, indicating it is selected.

Move the cursor into the viewing area. An image of the selected ring follows the cursor into the viewing area, replicating mouse movement. One atom in the ring is attached to the cursor.

1. Sketching 2D Molecules

Press and hold the left mouse button. The atom under the cursor provides an anchor point for the ring.

Continue to press and hold the mouse button as you move the cursor around the viewing area. The image of the ring rotates around the anchored atom as the image follows the cursor.

Release the mouse button. The ring is placed in the viewing area. The ring icon remains highlighted to indicate it is still selected.

2. Merge a second ring with the first ring.

Again, move the cursor in the viewing area. An image of a ring continues to follow the cursor.

Move the ring image over the ring already placed in the viewing area. The atoms in the placed ring are highlighted with a small square as the atoms in the ring image pass over them.

Move the ring image so two atoms are highlighted. Click the left mouse button. A second ring is merged with the first, joined at the bond between the two previously highlighted atoms. The ring icon remains highlighted to indicate it is still selected.

3. Turn off the ring selection.

Move the cursor over to the palette and the point icon. Click the left mouse button and the six-membered ring icon is no longer highlighted, indicating that the ring is no longer selected.

You can also turn off palette tools by positioning the cursor away from the structure in the viewing area and clicking the left mouse button twice.

Bonds

Bonds are selected from the palette by clicking on one of seven available bond icons. ChemNote automatically assigns carbon atoms to each bond as it is drawn, and supplies hydrogen atoms to meet valence requirements. As with rings, carbon and hydrogen symbols are not displayed by default. However, both can be displayed.

Single, double, and triple bonds are displayed by icons of solid single, double, and triple solid lines, respectively. Resonant bonds are represented by an icon containing a solid and a dotted line.

Since ChemNote requires all atoms to be associated with a structure, a coordination bond icon that contains a single dotted line can be used to con-

nect atoms that would normally exist without bond representation, for example, between sodium and the rest of the structure in sodium dodeca-sulphate.

Wedge bonds are used to define the relative position of side groups attached to an aliphatic ring. This allows you to position ring substitutes either axially or equatorially and build rings with substituents that are cis or trans to each other.

As described by IUPAC Rules and by Cahn, Ingold, and Prelog, filled wedge bonds extend from the display plane toward the viewer. Open wedge bonds extend from the display plane away from the viewer. The wide end of the wedge is closest to the viewer.

Using wedge bonds does not define chirality in ChemNote. You must specify R or S within atom properties for this purpose.

Use the next exercise to become familiar with using bond tools.

1. Add a bond to the rings.

Select the single bond icon and it becomes highlighted.

Move the cursor over the rings in the viewing area.

The atoms and bonds in the rings are highlighted with a small square as the cursor passes over them.

Move the cursor over the top-right atom in the structure and the atom is highlighted. Press and hold the left mouse button.

The message line displays:

Drag the mouse and release to place bond; double click the left button to exit.

Continue to press and hold the mouse button and move the cursor.

1. Sketching 2D Molecules

An image of the bond rotates around the anchor position, following the movement of the cursor.

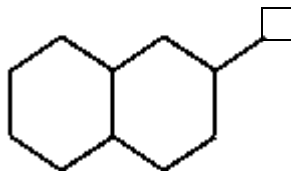
Release the mouse button and the bond is placed in the viewing area.

The single bond icon remains highlighted to indicate it is still selected.

2. Add a second bond

Move the cursor over the unanchored end of the bond just drawn and the atom is highlighted.

Press and hold the left mouse button. Move the cursor to position the bond image at an angle to the first bond. Release the mouse button and the second bond is placed in the viewing area.



The single bond icon remains highlighted to indicate it is still selected.

Move the cursor away from all objects placed in the viewing area, and quickly click the left mouse button twice.

The single bond icon is no longer highlighted, indicating the tool is no longer selected. The bond icon also can be turned off by selecting the point tool in the palette.

Changing atoms within a structure

It is possible to use atoms other than default carbon and hydrogen atoms. Using the mouse, you can select other elements from the Periodic Table and place them in structures. You can also choose to display undisplayed carbons and hydrogens.

Carbon substitution

Carbon atoms are automatically assumed to be bond endpoints and ring members. These atoms can be changed to any other element contained in the periodic table.

Complete the following exercise to practice making a carbon atom substitution.

1. Change a carbon atom to oxygen

Move the cursor over the symbol for oxygen located in the palette. Click the left mouse button and the **O** is highlighted to indicate it is selected.

Move the cursor over the rings and bonds in the viewing area.

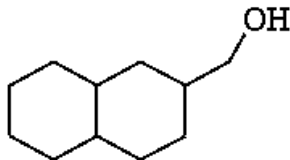
The atoms in the rings and bonds are highlighted with a small square as the cursor passes over them.

Move the cursor so that the atom located at the end of the second single bond is highlighted. Click the left mouse button.

1. Sketching 2D Molecules

The symbol OH is displayed near the atom, indicating the atom is now an oxygen automatically supplied with a hydrogen.

Select the point icon. The **O** tool is no longer highlighted, indicating the tool is no longer selected.



2. Display an undisplayed carbon atom.

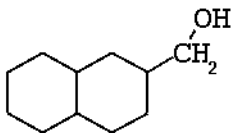
Move the cursor over the hydroxyl carbon and the atom is highlighted.

Click the left mouse button and move the cursor away from the atom.

The atom remains highlighted to indicate it is marked.

Display the **Layout** menu and select **Display Carbons**.

The symbol CH₂ is displayed near the marked atom indicating the atom is a carbon with two automatically supplied hydrogens. The atom remains marked.



Hydrogen atoms

Hydrogen atoms are automatically supplied to meet valence requirements as additional rings or bonds are drawn. The actual number of supplied hydrogens is determined by an atom's ionic charge.

Hydrogen atoms do not merge with nearby hydrogen atoms when a ring is placed. Dependent hydrogens are automatically deleted when their associated atoms or bonds are deleted. Bond placement does not allow attaching a bond to an automatically supplied hydrogen or replacing a bond attached to an automatically supplied hydrogen with a new bond.

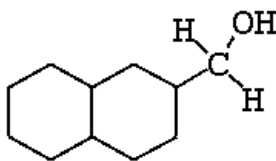
Complete the following exercise to become familiar with placement and display of hydrogens:

1. Change the display of the hydrogen atoms.

Display the **Layout** menu and select **Display H's**.

The symbol CH_2 is changed to C and the hydrogens are now displayed separately.

Display the **Layout** menu and select the **Suppress H's**.

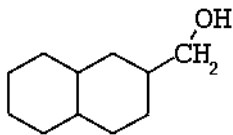


The hydrogen symbols are removed from the display. The carbon atom remains displayed as C.

Display the **Layout** menu and select **Abbreviate H's**.

The group symbol returns to CH_2 .

1. Sketching 2D Molecules



2. Remove the mark on the carbon atom

Move the cursor away from all objects in the viewing area and click the left mouse button.

This removes marks from all atoms and bonds.

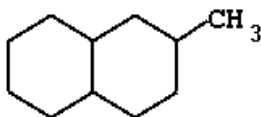
Marks also can be removed by selecting **Unmark All** from the **Edit** menu.

The carbon atom and attached hydrogens are no longer highlighted, indicating the group is no longer marked.

3. Delete the oxygen atom and bond

Mark the oxygen atom and select the Eraser tool. The oxygen atom and its bond connections are deleted.

The CH_2 group is changed to CH_3 , indicating another hydrogen was automatically added to the carbon when the OH group and bond were removed.



Customizing bonds

During the 2D to 3D conversion process, single or double bonds designated *cis/trans* or *axial/equatorial* are automatically placed correctly. Marking a bond and selecting either the **Cis/Trans** or **Axial/Equatorial** tools in the palette begin to cycle the bond through the available selections. Table 8, indicates the tools that are selected for each cycle.

Table 8. *Cis/trans* and *axial/equatorial* cycles

Cycle number	Cis/trans tool	Axial/equatorial Tool
1	Cis	Equatorial
2	Trans	Axial
3	None	None

You can determine what cycle these tools are in by the letter that appears in the middle of the bond. A marked bond will be identified by a *c* (*cis*), *t* (*trans*), *a* (*axial*) or *e* (*equatorial*) in the middle of the bond. A highlighted bond marked is opaque so it covers the bond indicator when it is activated. To see the indicator (*c*, *t*, *a*, or *e*), remove the highlighting by unmarking the bond.

Use the following exercise to practice marking bonds for the conversion process.

1. Defining the merged ring bond as *cis* or *trans*

Move the cursor over the common bond between the two rings in your structure.

The bond is highlighted.

Click the left mouse button, then move the cursor away from the bond.

1. Sketching 2D Molecules

The bond remains highlighted to indicate it is marked.

Select the **Cis/Trans** tool.

A *c* is displayed on the bond, indicating the bond is defined as *cis*. The bond remains highlighted, indicating it is still marked.

Again, select the **Cis/Trans** tool.

A *t* is displayed on the bond to indicate the bond is now defined as *trans*.

2. Unmark the merged ring bond.

Move the cursor over the shared bond and click the left mouse button.

The bond is no longer highlighted, indicating it is no longer marked.

Saving ChemNote structures

ChemNote allows only one structure to be saved at a time. It checks each sketch for the following before converting it to a 3D structure and saving it in a .mol file.

- Unattached atoms or bonds.
- Unknown CHARMM atom types.
- Net charge.

If a problem is found, ChemNote provides a dialog box prompt that identifies the problem and provides options for fixing it. For example, when a structure is saved, ChemNote checks that the total ionic charge of the structure is the same as the sum of the partial charges of the atoms. The net charge assignment number reported at the top of the dialog box represents the sum of the partial charges. The net charge number reported in the data entry field represents the sum of the ionic charges.

If the sum of the partial charges and the sum of the ionic charges are not the same, the dialog box provides several methods for adjusting partial charges.

After addressing these issues, ChemNote stores the 2D sketch in a .mol structure file. The application also creates a CHARMm RTF using the first four characters of the .mol filename as the RTF filename. To avoid ambiguity in RTF and residue naming, be sure that the first four characters of each .mol filename you create are unique. ChemNote checks against a list of known residues to prevent accidental duplication of names.

Use the following practice exercise to become familiar with the **Save** procedure.

1. Save a structure.

From the **File** menu, select **Save**.

A File Librarian is displayed.

Enter the name trans in the File Librarian filename field and click the **Save** button.

The File Librarian disappears from the screen and a dialog box appears.

2. Smooth the partial charges over the specified atoms.

ChemNote checks the net charge and finds it does not equal the sum of the individual partial charges of the atoms in this structure. A dialog box enables you to select a method for adjusting the partial charges.

Enter the default value in the charge field.

The dialog box reads:

The desired net charge is: 0.000

1. Sketching 2D Molecules

Chose the default option:

CT, CH1E, CH2E, CH3E, C5R, C6R, C5RE, C6RE, HA types

Click the **OK** button and the dialog box is closed.

The partial charges are changed, and new charges are saved in the trans.mol file. The sketch remains in the ChemNote window to provide the opportunity to use it as a base for creating another .mol file.

3. Change the merged ring bond to *cis*.

Mark the merged ring bond currently defined as *trans*.

Select **Cis/Trans** and the t displayed on the bond is removed, indicating that the bond is neither *cis* nor *trans*.

Again select **Cis/Trans**.

A c is displayed on the bond, indicating the bond is defined as *cis*.

Unmark the merged ring bond, and the bond is no longer highlighted.

4. Save the structure and smooth the partial charges.

From the **File** menu, select **Save**.

The File Librarian is displayed.

Enter the name *cis* in the File Librarian and click the **Save** button. Repeat the procedure in Step 2 for adjusting partial charges by selecting the default value and option in the dialog box that is displayed. Click the **OK** button to complete the procedure.

The dialog box is closed. The partial charges are changed, and new charges are saved in the *cis.mol* file. The sketch remains in the ChemNote window.

Returning to Molecular Modeling

When the 2D sketch is completed, the structure contained in the *.mol* file is brought into the Molecular Modeling application converted to a 3D *.msf* file for further modeling and analysis. The conversion is done automatically when you return to Molecular Modeling mode.

If an MSF is active in the viewing area of the molecule window, from previous work, a dialog box is displayed that presents options for displaying the structure converted from ChemNote.

Table 9 lists the options in this box and provides a brief description of each.

Table 9. Structure selection options

Option	Description
Use the new molecule filename only	Clears the viewing area of any structure(s) and displays only the structure in the new MSF.
Add this to your previous selection	Supplements the displayed structure(s) with the structure in the new MSF, maintaining the new MSF as a separate file.
Retain your previous selection	Maintains the displayed structure(s) in the viewing area and does not open the new MSF.

Use the following exercise to become familiar with the process of moving a structure from ChemNote to 3D Molecular Modeling mode.

1. Sketching 2D Molecules

1. Return cis.mol to Molecular Modeling.

Display the **File** menu and select **Return to Molecular Modeling**.

The ChemNote window is removed from the screen, revealing the Molecular Modeling window. The last saved structure in ChemNote, contained in the .mol file, is then automatically converted to an MSF.

2. Display cis.msf in Molecular Modeling

If you already have a structure displayed in the viewing area, a dialog box opens.

Select the default option **Use the new molecule cis.msf only** and click the **OK** button.

The structure is displayed in the Molecular Modeling viewing area. The Molecular Management Table is updated, and this information on the file is displayed in the textport:

```
31 atoms and 32 bonds read in
Setting bonding mode to use read-in connectivity
31 atoms selected for molecular structure cis.msf
31 atoms will be displayed
```

Importing a .mol file into Molecular Modeling

The **Import** selection in the **File** menu of the QUANTA menu bar allows you to import stored ChemNote .mol files. Complete the following exercise to become familiar with the import process.

1. Import the *trans* molecule into Molecular Modeling.

Display the **File** menu in Molecular Modeling mode and select **Import**.

A File Librarian dialog box lists the available external file formats and a scrolling list of available files of each format.

From the data format scrolling list, select **ChemNote**.

The top scrolling list and filename field change to reflect your selection. The scrolling list contains the .mol files that are available for selection.

Select the trans.mol file from the scrolling list and then select the **Import** button.

When the creation of trans.msf is complete, a dialog box is displayed so that the structure just created can be used.

Select the option **Add this to your previous selection** and click **OK**.

The structure trans.msf is added to the display of cis.msf in the **Molecular Modeling** viewing area. Information about the active molecules is displayed in the textport.

2. Move one MSF away from the other.

From the Modeling palette, select **Move Fragment**.

The message line reads:

Pick one atom - Reselect palette item tot qui. Pick atom to define center of moving fragment.

Pick any atom in the *cis* structure.

An ID is displayed next to the picked atom and the message line reads:
Fragment On

1. Sketching 2D Molecules

Undo Changes, **Save Changes**, and **Reject Changes** are activated in the Modeling palette. The Dial Emulator changes automatically to Dial Set 2.

Using the Y Translate dial, move the *cis* structure upward until it no longer overlaps the *trans* structure.

3. Save the new transformation of cis.msf

From the Modeling palette, select **Save Changes** and a dialog box offers saving options. Select the option **Select new generation of cis.msf** and click **OK**.

The textport reads:

The old structure file is renamed cis.msf,001.

The **Undo Changes**, **Save Changes**, and **Reject Changes** selections in the Modeling palette are dimmed, indicating there are no changes needing action. The Dial Emulator returns to its default setting.

4. Reset the display.

Move the cursor over the Reset View dial and click the left mouse button.

The structures in the viewing area are repositioned. Both structures are now visible, and the conformational differences are easy to see.

Using templates

A template is any single connected structure of atoms and bonds that can be used as a building block for creating a new chemical structure. Templates are stored in standard ChemNote .mol files, each file containing one or more templates.

Templates allow chemical structures to be copied from the Template window and pasted into an existing sketch. The cut-and-paste procedure uses a clipboard that provides temporary storage for a template. The clipboard subdirectory is automatically created under your home directory. When a template is placed in the clipboard, it can be incorporated into the viewing area with the **Paste** selection from the ChemNote **Edit** menu.

The Template window

The **Template** function opens from the ChemNote **File** menu. When it is selected, the Template window opens over the ChemNote window. Since you work in both windows to build a structure using a template, position the windows so both are visible on your screen.

The template window has five distinct areas:

- Menu bar
- Title bar
- Buttons
- Command line
- Message line

Although some window areas are the same as in other QUANTA applications, the menu bar, title line, and buttons are specifically customized for the Template Viewer.

Title bar

The title bar appears at the top of the window and contains the name of the current template file and the minimize/maximize button.

Menu bar

The menu bar contains three menus. Menu names and a brief functional description are listed in [Table 10](#). Template menus are displayed as pull-down or sticky menus.

Buttons

The buttons allow the keyboard to be used instead of the mouse for selecting a template, by entering an atom or element name in the data entry field located to the right of the buttons.

1. Sketching 2D Molecules

Table 10. Menu bar

Menu	Description
File	Opens any .mol file for display in the template window. Views the contents of the clipboard. Exits the Template Viewer.
Template	Displays an alphabetical list of available template files for direct access. Template files contained in this list are located in the subdirectory QNT_CHEM/templates.
Help	Provides software copyright and version number information. Accesses on-line help.

The **Search** button looks through the template file for the atom name that was entered in the data entry field, highlights the atom, and copies the template containing that atom to the clipboard. If there is more than one template with an atom of that name, the first one encountered is copied. If a name is not found, a message is displayed. The **Clear** button erases any text from the data entry field.

Building a template-based structure

The following exercise involves building Orange II, the sodium salt of 4-(2-hydroxy-1-naphthylazo) benzenesulfonic acid. Use this example to become familiar with the template, the editing, bonding, and atom functions, and the tools in ChemNote. Because of the ionic bond that sodium forms with the organic sulfate, the exercise also demonstrates the use of multiple MSFs.

This procedure creates the components for Orange II and then imports the structure to Molecular Modeling, where the CHARMM energy can be calculated.

1. Start ChemNote and the Template Viewer

In the Molecular Modeling window, display the **Applications** menu. Select **Builder** and then **2D Sketcher** from the pull-right menu.

The ChemNote window is displayed.

In the ChemNote window, open the **File** menu and select **Template**.

The Template Viewer window is displayed over the ChemNote window.

By default, a selection of carbocyclic group templates are displayed.

Move the ChemNote and Template Viewer windows so the viewing areas of both are visible.

2. Select naphthalene from the Template Viewer window

Move the mouse so that the cursor is located in the Template viewing area. Move the cursor over an atom in the naphthalene structure and the atom is highlighted with a small square.

Click the left mouse button.

The message line reads:

Copying...

indicating that the naphthalene structure is being copied to the clipboard. When the process is complete, the message line reads:

Structure copied to clipboard.

Move the mouse so the cursor is located in the ChemNote window. Display the **Edit** menu and select **Paste**.

The naphthalene structure is displayed in the center of the ChemNote viewing area.

The pasted structure may not be visible if the Template Viewer window is displayed over the center of the ChemNote viewing area.

Move the structure by placing the cursor over any atom or bond and pressing and holding the left mouse button while moving the mouse. To release and place the structure, release then click the mouse button.

1. Sketching 2D Molecules

Select **Rotate** on the palette to rotate the structure counterclockwise 90° to a vertical position.

Using the Point icon, drag a box around the naphthalene molecule selecting all its atoms. Then from the **Layout** menu select **Atom Name**.

All of carbon atoms in the molecule will be shown in their numbered sequence. Numbering is according to the build sequence for the molecule.

3. Add nitrogen to the structure.

With the single bond icon on the palette, add a single bond to the C10 carbon.

Select **N** from the atom tools portion of the palette. Click the new carbon, changing it to a nitrogen.

Select the double bond icon and add a double bond to the nitrogen.

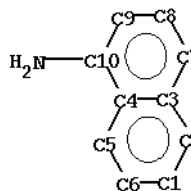
Select **N** again and click the new carbon at the end of the double bond, also changing it to nitrogen

4. Select and paste benzenesulfonic acid into ChemNote

The atom is highlighted with a small square.
The message line reads:

Copying

indicating that the benzenesulfonic acid structure is being copied to the clipboard. When the copy is complete, the message line reads:



Return to the Template Viewer window. From the **Template** menu, select **Functional_Groups-2**.

Move the mouse so that the cursor is located in the Template viewing area. Move the cursor over an atom in the benzenesulfonic acid structure.

Click the left mouse button.

Structure copied to Clipboard

Move the mouse so the cursor is located in the ChemNote window. Display the **Edit** menu and select **Paste**.

The benzenesulfonic acid structure is displayed in red in the center of the ChemNote viewing area.

Position the two structures so that the final nitrogen of the parent naphthalene structure and the nonsulfonic carbon of the benzenesulfonic acid structure are aligned end to end. Click the left mouse button to connect the two structures. Make sure the structures are bonded correctly.

1. Sketching 2D Molecules

5. Select all atoms

Using the Point icon, drag a box around the naphthalene molecule, selecting all its atoms. Then from the **Layout** menu, select **Atom Name**.

All the nonhydrogen atoms in the molecule are shown in their numbered sequence.

6. Close the Template Viewer window

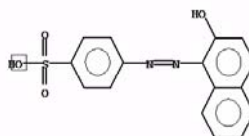
Move the mouse so the cursor is located in the Template Viewer window. Display the **File** menu and select **Quit**.

The Template Viewer window is removed from the screen.

7. Add additional oxygens to the structure

Move the mouse so the cursor is located in the ChemNote window. Select the single bond icon and add a single bond to the C9 carbon on the parent naphthalene structure.

Select the oxygen symbol from the atom selections. Click the new carbon changing it to oxygen.



A hydrogen is automatically supplied, creating an OH group.

With the **O** symbol still selected, click the **C** of the sulfonic acid group, substituting an oxygen.

8. Assign partial and ionic charges

Double click the new oxygen atom that is part of the sulfonic acid group. A dialog box for assigning properties opens. This box also can be opened by selecting **Atom Properties** in the **Properties** menu.

Select the following options:

Ionic Charge: -1

Partial Charge: -1.000 Lock

Ignore Valence Check: Yes

Click the **OK** button.

9. Return to Molecular Modeling.

Display the **File** menu and select **Return to Molecular Modeling**. Since the Orange structure has not been saved to a file, a dialog box asks if the changes are to be saved. Select the **Yes** button.

In the File Librarian dialog box that opens, enter the name **orange** and click the **Save** button.

In another dialog box that prompts you to select the method for adjusting partial charges, enter the value: **The desired net charge is: -1.000.**

1. Sketching 2D Molecules

Select the following option **CT, CH1E, CH2E, CH3E, C5R, C6R, C5RE, C6Re, HA types** and click the **OK** button.

The ChemNote window is removed from the screen, revealing the Molecular Modeling window and a dialog box.

Select the option **Use the new molecule orange.msf only** and click the **OK** button.

If any structures were displayed in the Molecular Modeling viewing area, they are removed and replaced by the structure orange.msf.

10. Return to ChemNote and create the ion file sodium.msf

In the Molecular Modeling window, display the **Applications** menu.

Select **Builder** then **2D Sketcher** from the pull-right menu.

The ChemNote window is displayed.

Click the **Periodic Table** icon and select the **Na** symbol. Click the **OK** button

With the mouse, move the cursor to the ChemNote window and click on the screen, placing the sodium atom.

Select the point tool. The Periodic Table is no longer selected.

11. Assigning ionic charge

Double-click the sodium atom, and the Assign Properties dialog box is displayed. Select the following options:

Ionic Charge: 1

Ignore Valence Check: Yes

Click the **OK** button.

12. Return the sodium ion to Molecular Modeling

Display the **File** menu and select **Return to Molecular Modeling**. Since this fragment has not been saved to a file, a dialog box asks if the changes are to be saved.

Click the **Yes** button and the File Librarian is displayed.

Enter the name **sodium** in the File Librarian and then click the **Save** button. A dialog box prompts you for the method for adjusting partial charges.

Enter the value **The desired net charge is: +1.000**.

Select the following option **CT, CH1E, CH2E, CH3E, C5R, C6R, C5RE, C6Re, HA types** and click the **OK** button.

1. Sketching 2D Molecules

The ChemNote window is removed from the screen, revealing the Molecular Modeling window and a dialog box.

Select the option **Add this to your previous selection** and click the **OK** button.

The ion sodium.msf is added to the Molecular Modeling viewing area along with orange.msf, and information on the structure is added to the Molecule Management table. A hydrogen has been removed from the sulfide group as a result of the charge adjustments made to the Orange molecule.

To close the files, go to the **File** menu and select **Close**.

A dialog box allows you to choose the files you want to close.

Select the **Close All** button between the two scrolling lists. Both MSFs are moved into the **Close** scrolling list. Click the **OK** button.

Both structures are removed from the viewing area and saved in their respective MSFs. You will use them again in later chapters.

Summary

ChemNote is QUANTA's 2D molecular sketching application. The application runs in a separate window that is opened over all QUANTA windows. Other activity in QUANTA is frozen until ChemNote is closed.

In ChemNote, sketches are created by progressively selecting and positioning various rings, bonds, and atoms or by selecting and modifying templates supplied with the application. Templates are accessed through a template window.

Chemical properties such as partial atomic charges, saturation, chirality, isotopes, and *cis/trans* and axial/equatorial geometry can be assigned in ChemNote. The application also provides control over the display of carbons and hydrogens within the sketch.

Any 2D sketch created in ChemNote is automatically converted to a 3D structure in a .mol file when the structure is moved into the Molecular Modeling application. ChemNote creates a .pct file that saves the 2D graphical data for continued use within ChemNote. The application also creates an RTF that is used by CHARMM to generate a PSF. The ChemNote .mol file automatically converts to an MSF when ChemNote is closed and Molecular Modeling reactivated. This conversion also occurs when an existing .mol file is imported into Molecular Modeling.

1. Sketching 2D Molecules

2. Editing 3D Structures

This chapter describes the basics of using the QUANTA Molecular Editor for editing 3D structures and preparing them for various operations and calculations. It also includes a description of additional editing options, including the Atom Property Editor available on the **Edit** menu in the Molecular Modeling menu bar. This chapter should be read by all QUANTA users.

The Molecular Editor provides tools to construct and modify any 3D molecular structure. The application's basic editing capabilities provide ways for you to add or delete atoms, change atom types, and build a structure by merging a number of molecular fragments.

If you want to combine structures stored in more than one MSF into a single MSF, open the files *before* you enter the Molecular Editor. Use the **Save As** selection in the Molecular Modeling **File** menu to combine the structures into a single MSF.

The Molecular Editor also prepares a structure for CHARMM operations. It assigns atom types and charges to all atoms and satisfies valence requirements by adding hydrogens to the structure during editing procedures.

When you exit the Molecular Editor, a final valence check is automatically performed to minimize inconsistencies that may have occurred during editing. A single MSF is created even if multiple fragments exist. You also may choose to create a CHARMM RTF for a single fragment. After the MSF and any optional RTFs are created, QUANTA returns to the Molecular Modeling application.

The **Edit** menu includes other editing options including **Bond Options**, **Atom Data**, and the **Atom Property Editor**. Each of these operates on molecular properties defined in an MSF.

Creating a base structure

Although the Molecular Editor allows 3D structures to be built by merging a number of molecular fragments, it is often faster and easier to sketch the base structure in ChemNote. This approach also may provide a more accurate structure for beginning your 3D editing procedures.

ChemNote checks each sketch for unattached atoms or bonds, unknown CHARMM atom types, and net charges before 3D conversion takes place. If any inconsistency is found, a dialog box is displayed that identifies the

2. Editing 3D Structures

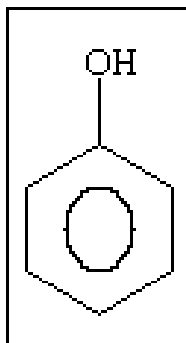
problem and provides a set of options for resolving it. Only when the 2D sketch is verified as correct, does ChemNote convert it into a 3D structure file.

Use the following exercise to create a base structure for editing in the Molecular Editor. If you have not built 2D molecules in ChemNote, go through chapter 1 of this volume before continuing.

1. Create phenol in ChemNote

In the Molecular Modeling window, display the **Applications** menu. Select **Builders**, then select **2D Sketcher** from the pull-right menu and the ChemNote window is displayed.

Sketch the structure phenol and save it as phenol.mol.



2. Return the phenol structure to Molecular Modeling

Display the **File** menu in the ChemNote window and select **Return to Molecular Modeling**. A dialog box asks if the changes made are to be saved.

Click the **Yes** button and a File Librarian dialog box is displayed.

Enter the name **phenol** in the dialog box and click the **Save** button.

The ChemNote window is removed from the screen and the Molecular Modeling window is reactivated.

The phenol.mol file is automatically converted to the MSF phenol.msf. A dialog box gives you the choice of using either the structure that was just created or another MSF. Select the option:

Use the new molecule phenol.msf only and click **OK**.

The structure phenol.msf is displayed in the viewing area. The textport message indicates that 13 atoms are active, and the Molecule Management Table displays the status of phenol.msf.

editing
3D

Editing bonds and fragments

The Molecular Editor provides tools for editing bonds and molecular fragments. Some of these editing tools include functions such as adding and deleting bonds and fragments, replacing and merging fragments, and changing bond types.

Editing tools are located in the Molecular Editor palette that opens when you select **Molecular Editor** from the **Edit** menu in the menu bar. This palette can also be accessed through the **Applications** menu in the menu bar by selecting **Builders** and then **3D Builder** from the pull-right menu.

The palette functions like other QUANTA palettes. When a selection is chosen, it is checked and highlighted to indicate it is active. Some selections remain active until they are manually turned off or until another selection is made. Other selections are automatically turned off when the associated function is complete.

[Table 11](#) lists the Molecular Editor palette selections with a brief description of each.

Table 11. Molecular Editor palette

Selection	Description
Display Atom Labels	Labels all atoms each time the tool is selected, using the following cycle: atom names, residue names, atom types, atom charges, no labels.
Add Atoms	Toggles the display of the Add Atoms palette, which provides tools to add atoms or functional groups to the molecular structure.
Change Atoms	Changes the selected atom to the user-specified element. The atom number is automatically appended to the element name to generate a new atom name to guide subsequent atom typing.
Edit Atoms	Toggles the display of the Edit Atoms palette that has a variety of editing selections for atoms.
Delete Atoms	Removes selected atoms and their associated bonds from the molecular structure. Deleting an atom may generate a fragment. This selection can be used to delete a single atom fragment.
Add Bond	Creates a bond between two selected atoms. If a bond exists between the picked atoms, the application asks for information on the bond type of the new bond (single, double, triple, aromatic). Minimization can correct improper bond lengths and angles.
Change Bond	Changes bond types each time the tool is selected using the following cycle: single, double, triple, aromatic. The selected bond is set to the next bond type in the cycle.
Edit Bonds	Toggles the display of the Edit Bonds palette that has a variety of editing selections for bonds.
Swap Bonds	Interchanges selected bonds.
Torsions	Modifies the structure by torsional rotations around a set of user-specified bonds.
Delete Bond	Removes a selected bond from the structure, possibly creating a new fragment.
Display Fragment Table	Displays the Fragment and Categories tables. Through toggle selection, one or more fragments can be placed in the active MSF displayed in the viewing window.
Move Fragment	Allows a fragment to be moved using any of the X, Y, Z translate or rotate dial emulators. Only one fragment can be moved at a given time. Selecting a new palette tool automatically saves the current transformation of a fragment.
Merge Fragments	Joins two fragments after selecting one bond in each fragment. This tool only operates on terminal bonds.
Replace All With Fragment	Removes all displayed molecular structures from the viewing area and allows a new fragment to be read into the application.
Delete Fragment	Removes a selected fragment from the viewing area.
Add All Hydrogens	Satisfies valence requirements based on atom type by adding hydrogens to all atoms. Atoms are not retyped automatically. In the Edit Atoms palette, use Type All Atoms for correct atom type assignments.
Add Polar Hydrogens	Adds hydrogens to all oxygen and nitrogen atoms. Atoms are not retyped automatically. In the Edit Atoms palette, use Type All Atoms for correct atom type assignments.
Delete Hydrogens	Deletes all hydrogen atoms from the molecular structure. Atoms are not retyped automatically. Use Type All Atoms for correct atom type assignments.

Table 11. Molecular Editor palette

Selection	Description
CHARMm Mini- mize	Minimizes the current structure in the viewing area.
Editor Options...	Displays the dialog box from which the Molecular Editor defaults can be changed. The Keep Display Selection option allows a display mask set from Molecular Modeling to be maintained in the Molecular Editor.
Undo	Undoes the last edit operation. The number of steps which can be undone is controlled by the Maximum number of UNDO steps field in the Editor Options dialog box. If there are no more steps which can be undone, the Undo tool is masked.
Revert to Initial Structure	Restores the structure as it was on entering the molecular editor.
Quit	Exits the Molecular Editor without saving any changes made during editing.
Save and Exit	Exits the Molecular Editor and returns to the Molecular Modeling application. The structure is saved according to current save options.

Use the following exercise to become familiar with the Molecular Editor.

1. Start the Molecular Editor

Display the **Edit** menu and select **Molecular Editor**. The Molecular Editor palette replaces the Molecular Modeling palette.

2. Change a bond in the phenol ring

Select **Change Bond** from the palette.

The message line prompts:

Pick bond to change.

Position the cursor over any bond in the phenol ring. Click the left mouse button. The bond is briefly highlighted, indicating it is selected, and it changes from an aromatic bond to a single bond.

2. Editing 3D Structures

Select the bond again and the bond changes to a double bond.

Cycle through the remaining bond types by selecting the bond two more times.

It changes to a triple bond and then back to an aromatic bond.

3. Change the display to a Kekule Structure

Select **Edit Bonds** in the Molecular Editor palette to open the Edit Bonds palette.

See [Table 12](#) for a list of selections in the Edit Bonds palette and a brief description of each.

Select **Display Kekule Structures**. The bonds in the aromatic ring change to alternating double and single bonds. Select **Display Kekule Structures** again. The display returns to aromatic bonds.

Select **Exit Edit Bonds**. The Edit Bonds palette is removed from the screen.

4. Add a fragment to the MSE.

The message in the textport reads:

```
Adding fragment .../quanta/fragment/propyl.mol
```

The number of atoms listed in the Molecule Management table changes to 24.

5. Merge the propyl fragment with the phenol ring

The Move Fragment dials are automatically closed and the message line reads:

Table 12. Edit Bonds palette

Selection	Description
Set Bond Length	Adjusts the length of any bond that is not part of a ring
Set Bond Angle	Adjusts the angle between two adjacent bonds that are not part of a ring.
Set Torsion Angle	Sets a user-specified dihedral or improper dihedral angle.
Aromatize/Dearomatize	Toggles bond types of a ring from single to aromatic or visa versa, depending on initial bond type. Retypes atoms accordingly. Hydrogens are not added or deleted by this operation, nor is the geometry of the ring modified. The Add All Hydrogens selection in the Molecular Editor palette may be used to saturate a ring.
Display Kekule Structures	Toggles rings with aromatic bonds to rings linked by alternating single and double bonds or visa versa, depending on initial ring type.
Set Bond Types By Distance	Toggles the bond type by bond distances.
Set Bond Types By Atom Type	Toggles the bond type by atom type.
Exit Edit Bonds	Exits the Edit Bond palette.

Select **Display Fragment Table** from the Molecular Editor palette and the Fragment and Categories Tables open on the left of the viewing area. A number of categories of fragments are available in a scrolling list in the Categories Table.

Select the category **Functional Groups** and the Fragment Table displays functional group fragments in a scrolling list. If you click **Toggle Icons** at the top of the table, the list displays both the name and a chemical representation of each fragment.

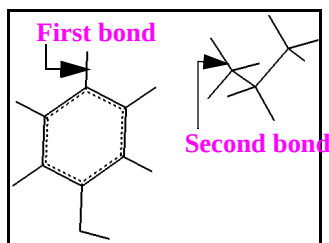
Click the **propyl** fragment in the Fragment Table and a propyl fragment is added to the viewing area. Click only once since additional clicks add additional propyl fragments.

Again click **Display Fragment Table** to deselect it. The Fragment and Categories Tables are removed from the screen.

2. Editing 3D Structures

Select **Move Fragment** from the Molecular Editor palette then select any atom in the propyl fragment. Use the translate and rotate dials in the Dial Emulator to position the fragment so that the propyl structure is fully visible relative to the phenol structure.

Select **Merge Fragment** from the Molecular Editor palette.



Pick the first bond to merge.

Pick the bond between the para carbon and hydrogen in the phenol ring.

The bond is briefly highlighted, indicating it is selected, and the message line reads:

Pick the second bond to merge.

Pick a bond between a terminal carbon and a hydrogen in the propyl fragment.

The selected bonds are joined, merging the propyl fragment with the phenol ring. The selection is automatically turned off when the merge operation is completed. The number of atoms listed in the Molecule Management Table now reads 22, because two atoms were eliminated in the merger.

6. Rotate the structure for better visibility

Press and hold the middle mouse button while moving the mouse to rotate the structure until all bonds can be seen. Release the mouse button and the structure stops rotating.

Customizing the Fragment Table

The Fragment Table can easily be customized to contain your own fragments, in the form of ChemNote .mol files, or to present the categories in a different order if you use some more often than others.

Make a copy of the file \$HYD_LIB/fragment.lib. Make this copy editable (**chmod u+w fragment.lib**) and read it into an editor. Add a line consisting of the pathname of a directory containing a collection of .mol files, followed by a description. You can add as many lines as you wish if you want to organize your fragments into separate directories to constitute your own categories, and rearrange or even comment out any of the standard categories you don't want to use

Your modified fragment.lib file can be placed either in the directory from which you run Quanta, or you may wish to create a directory containing this and other default files which can be anywhere, pointed to by an environment variable QNT_USR.

If you want to minimize the coordinates in your .mol files, without altering the 2D coordinates which are used to draw the icons in the fragment table, there is an unsupported utility available accessed by the command Z118.

editing
3D

Altering atoms

There are several options for adding, changing, and editing atoms in the Molecular Editor. You can add or modify oxygen, carbon, or hydrogen by using the **Add Atoms** selection in the Molecular Editor palette. When you select **Add Atoms**, a palette is displayed. Table 14, lists the **Add Atom** selections and briefly describes each.

If you want to make changes with elements other than hydrogen, carbon, or oxygen, use **Change Atoms** in the Molecular Editor palette. This selection opens a dialog box where you enter the element of your choice.

Table 13. Add Atoms palette

Selection	Description
Add H to sp3	Adds a hydrogen atom to an sp3 target atom, placing the new atom at 109.47° to the existing bond.
Add H to sp2	Adds a hydrogen atom to an sp2 target atom, placing the new atom at 120° to the existing bond.
Add H to sp1	Adds a hydrogen atom to an sp1 target atom, placing the new atom at 180° to the existing bond.
Add C to sp3	Adds a carbon atom to an sp3 target atom, placing the new atom at 109.47° to the existing bond.
Add C to sp2	Adds a carbon atom to an sp2 target atom, placing the new atom at 120° to the existing bond.
Add C to sp1	Adds a carbon atom to an sp2 target atom, placing the new atom at 180° to the existing bond.
Add O to sp3	Adds an oxygen atom to an sp3 target atom, placing the new atom at 109.47° to the existing bond.
Add O to sp2	Adds an oxygen atom to an sp2 target atom, placing the new atom at 120° to the existing bond.
Convert to Methyl	Converts the selected atom to a methyl group. The selected atom is converted into a tetrahedral carbon atom, and three hydrogens are added at tetrahedral positions.
Convert to Hydroxyl	Converts the selected atom to a hydroxyl group. The selected atom is converted into an oxygen atom, and a hydrogen is added to it at a tetrahedral angle.
Convert to Amine	Converts the selected atom to an amine group. The selected atom is converted to a tetrahedrally coordinated nitrogen atom, with two hydrogen atoms attached.
Convert to Amide	Converts the selected atom to an amide group. The selected atom is converted into a planar nitrogen atom, with two hydrogen atoms attached.
Convert to Carbonyl	Converts the selected atom to a carbonyl group. The selected atom is converted into an sp2 carbon atom, and a double-bonded oxygen and a hydrogen atom are attached.
Exit Add Atoms	Removes the Add Atoms palette from the screen.

You can edit atoms singly or in groups by using the **Edit Atoms** selection in the Molecular Editor palette. When you select **Edit Atoms**, a palette is displayed. Table 14, lists the selections on this palette and provides a brief description of each.

New atoms are named by adding a sequential number to the element name (O1, O2, O3, H1, H2, H3). An automatic renaming procedure executes when you exit the Molecular Editor to ensure atom name uniqueness. This procedure is selected as a default in the Editor Options dialog box.

Atom names as well as other important information about each atom in the structure are used as atom labels by selecting **Display Atom Labels** from

Table 14. Edit Atoms palette

Selection	Description
Set Atom Type...	Requests an atom pick for type setting, then displays a dialog box with type, filter, and lock choices.
Type All Atoms	Types all atoms in the molecule using CHARMM-based templates.
Set Atom Charge	Opens a Select palette for choosing atoms to charge.
Charge All Atoms	Displays a dialog box allowing you to choose the charge template or Gasteiger method for determining the charge.
Report Total Charge	Reports total molecular charge in textport.
Rename Atoms	Requests that you pick specific atom(s) to be renamed. Opens dialog box with new name field.
Rename Residue	Requests that you pick specific residue(s) to be renamed. Opens dialog box with new name field.
Edit Coordinate	Opens a coordinate table. Edit coordinates directly using the table Edit menu and table editing functions.
Invert Z Coordinates	Repositions structure with respect to the z axis.
Report Chirality	Requests that you pick a chiral center. After center is picked, chirality is reported in the Textport.
Exit Edit Atoms	Exists the Edit Atoms palette and redisplay the Molecular Editor palette.

the Molecular Editor palette. This selection provides atom label information each time it is used in the following cycle: atom names, residue names, atom types, atom charges, no labels

Three tools are provided in the Molecular Editor palette for working with hydrogen.

- The **Add All Hydrogens** selection satisfies valence requirements by adding hydrogens to all atoms. Valence requirements are determined by bond type
- The **Add Polar Hydrogens** selection adds hydrogens to all oxygen and nitrogen atoms.
- The **Delete Hydrogens** selection deletes all hydrogen atoms from the molecular structure.

Altering the molecular structure by adding or deleting hydrogens as well as making other structural changes requires atoms to be retyped. There are two typing procedures: automatic and manual. Automatic typing is done when you exit the Molecular Editor. If the parameters you are using differ from the defaults, they need to be redefined.

You initiate manual retyping by selecting **Type All Atoms** in the Edit Atoms palette that opens when you select **Edit Atoms** from the Molecular Editor palette.

2. Editing 3D Structures

Complete the following exercise to become familiar with procedures for adding or modifying oxygen, hydrogen, or carbon atoms to a structure.

1. Display atom labels

Select **Display Atom Labels** from the Molecular Editor palette to cycle through the various label options: atom name, residue name, atom type, atoms charge, or no label.

Each time the selection is chosen, the labels cycle to the next option. Cycle through until you return to the atom name option.

2. Display the Add Atoms palette

Select **Add Atoms** from the Molecular Editor palette and the Add Atoms palette opens over the Molecular Editor palette.

3. Convert a hydrogen to a hydroxyl group

Select **Convert to Hydroxyl** from the Add Atoms palette.

The message line reads:

Pick atom to convert

Select the ortho hydrogen atom and the atom changes to a hydroxyl group.

4. Convert a hydrogen of the terminal methyl group to an amine group

Select **Convert to Amine** from the Add Atoms palette.

The message line reads:

Pick atom to convert

Select a hydrogen atom in the terminal methyl group and the atom is changed to an amine group.

The geometry is regularized for the MSF.

5. Exit the Add Atoms palette.

Select **Exit Add Atoms** from the Add Atoms palette.

The palette is removed from the screen.

6. Display atom types information in the atom labels.

Select **Display Atoms Labels** from the Molecular Editor palette and the labels change from atom names to residue names. Choose the selection again and the labels change from residue names to atom types.

7. Delete two methylene hydrogens from the alkyl chain

Select **Delete Atoms** from the Molecular Editor palette.

The message line reads:

Pick an atom to delete

Select the two methylene hydrogens in the alkyl chain and these atoms are removed from the structure.

The atom type changes from CT to CH2E for the carbon in the alkyl chain where the hydrogen atoms were deleted automatically.

8. Add hydrogens back to the structure.

Select **Add All Hydrogens** from the Molecular Editor palette.

Hydrogen atoms are added back to the structure, satisfying valence requirements. The atom type automatically changes from CH2E back to CT for the carbon in the alkyl chain where the hydrogen atoms were added.

Minimizing a structure

Structures created with the Molecular Editor may not have accurate geometries including bond lengths and bond angles. These geometries can be refined using an energy minimization process before you exit from the Molecular Editor. The process is initiated by selecting **CHARMm Minimize** from the Molecular Editor palette.

The energy minimization process also may be initiated by selecting **CHARMm Energy** from the Modeling palette. Chapter 3, *Calculating and Minimizing Energy*, is devoted to a more extensive description of energy minimization.

The following exercise goes through the minimization process as it is executed from within the Molecular Editor.

1. Setup minimization for the displayed structure.

Display the **CHARMm** menu and select the **Minimization Options** function.

In a dialog box containing minimization setup options, select the option **Steepest Descents**

For each data field, enter the values indicated:

Number of Minimization Steps: 50
Coordinate Update Frequency: 5
Energy Gradient Tolerance: 0.010000
Energy Value Tolerance: 0.000000
Initial Step Size: 0.020000
Step Value Tolerance: 0.000000

and click the **OK** button.

The dialog box is cleared from the screen and new minimization parameters are established.

2. Start minimization for your structure.

Select **CHARMm Minimize** from the Molecular Editor palette.

As the CHARMm calculation starts, the cursor changes from an arrow to a clock. The message line and textport display minimization information during the CHARMm process.

Minimization is completed when the cursor is restored to an arrow. The minimized energy result is displayed in the upper- right corner of the viewing area and reported in the textport.

If you wish to repeat minimization using another minimization method, repeat Steps 1 and 2, making selections appropriate for the method you choose.

Saving a structure

When you exit from the Molecular Editor, your structure is saved using options specified in the Editor Options dialog box. These options specify whether atoms are retyped or renamed, if charges are assigned, or if an RTF is created.

Charges are assigned using QUANTA charge templates or the Gasteiger method. The charge templates are derived from the CHARMm RTFs used for proteins and peptides. The templates have been expanded to include drug ligands and some polymers. In general, charge templates can be used

2. Editing 3D Structures

for any molecule that can be successfully typed in the Molecular Editor. Gasteiger charge methods should be applied to molecules that cannot be typed by in the editor.

The Editor Options dialog box is displayed when you select **Editor Options** from the Molecular Editor palette. By selecting **Prompt for Options during Exit** in the dialog box, you choose to have a similar dialog box displayed each time **Save and Exit** is selected from the Molecular Editor palette.

Table 15 summarizes the **Editor Options** listed in the dialog box..

Table 15. Molecular Editor options

Option	Description
Structure Regularization options	
Retype Changed Atoms/ Reassign	Automatically retypes all atoms when you save the molecular structure. Default option.
Automatically Adjust Bond Lengths	Automatically adjusts bond lengths when you save the molecular structure.
Automatically Optimize Angles	Automatically optimizes angle values when you save the molecular structure
General Options	
Keep Display Selection when Entering Editor	Retains display format chosen prior to performing editing procedures.
Maximum Number of UNDO Steps	Specifies the maximum number of edit operations which can be undone.
First-picked Fragment in Merge stationary instead of the larger	If this box is checked, then when merging two fragments, the second one picked will move to join the first picked. Otherwise, the smaller fragment will move to the larger one.
Exit options	
Reassign Atom Types	Assigns appropriate atom types to atoms that are changed during editing. Does not retype locked atoms.
Remove Locks on Atom Types	Removes atom type restrictions.
Reassign Atom Charges	See next two choices.
Use Charge Templates	Assigns charges to atoms using the charge template method. Atom types, locked with the Set Atom Charge selection in the Molecular Editor Options palette, are not recharged. Default option.
Use Gasteiger Method	Assigns charges to atoms using the Gasteiger method. Atom types, locked with the Set Atom Charge selection in the Molecular Editor Options palette, are not recharged.

Table 15. Molecular Editor options (Continued)

Option	Description
Rename Atoms Automatically	Renames all atoms during the save and exit procedure by concatenating the element name and the atom number to generate a unique name.
Generate RTF	See next two choices.
Single Residue	Creates an RTF when the structure is saved, modifying the structure so all atoms are contained in a single residue. Default option. This option should not be used for structures with multiple residues.
Peptide Residue	Creates a new RTF for each changed peptide residue (containing connected atoms named N, C α , and C) in the structure. All non-peptide residues bonded to a peptide residue are merged into the single peptide residue.
Prompt for Options during Exit	Displays a dialog box specifying save options each time Save and Exit is selected from the Molecular Editor palette.

The following exercise takes you through the **Save and Exit** procedure.

1. Save the structure and exit the Molecular Editor

Select **Save and Exit** from the Molecular Editor palette and a dialog box displays the default saving options:

Reassign atom types

Reassign atom charges - Use Charge Templates

Rename Atoms Automatically During Exit

Select the **OK** button.

A dialog box prompts you to choose the method for adjusting charges.

In the **Total Charge** data field, enter the value **0.0000**

Select the option **Carbon and nonpolar hydrogen** and click the **OK** button.

In the Saving Options dialog box, select **Save to New Filename**.

In response to a prompt from a File Librarian dialog box, enter the name **search1** in the filename data field and click the **Save** button.

The Modeling palette replaces the Molecular Editor palette.

Saving and exiting with multiple structures

You can work on several structures at the same time. When you have multiple MSFs open in the Molecular Editor, the final Save Options dialog box differs from the one displayed when you save a single MSF.

If you want to combine structures stored in more than one MSF, open the files *before* you enter the Molecular Editor. Use the **Save As** selection in the Molecular Modeling **File** menu to combine the structures into a single MSF. Then proceed to editing.

The following exercise creates an additional structure and MSF using ChemNote and the Molecular Editor, then leads you through the save and exit process with several MSFs.

1. Create methanol in ChemNote

Display the **Applications** menu. Select **Builders** and then **2D Sketcher** from the pull-right menu that opens.

In the ChemNote window that opens, sketch the structure methanol (CH_3OH) and save it as methanol.mol.

2. Return the methanol structure to Molecular Modeling.

Display the **File** menu in ChemNote and select **Return to Molecular Modeling**.

A dialog box asks if the changes made are to be saved.

Click on the **Yes** button.

A File Librarian dialog box opens.

Enter the name **methanol** and click the **Save** button.

In the smoothing dialog box, the smoothing algorithm adjusts the net charge to zero using the atoms you select.

Accept the default values by selecting **OK** to continue.

The ChemNote window is removed from the screen and the Molecular Modeling window is reactivated.

The file methanol.mol is then automatically converted to the MSF file methanol.msf. A dialog box gives you the options of using either the structure that was just created, another MSF file, or one added to the other.

Select the option **Add this to your previous selection** and click the **OK** button.

The structure methanol.msf is displayed along with search1.msf in the viewing area. The textport message indicates that 31 atoms are active. The Molecule Management Table displays the status of both search1.msf and methanol.msf.

3. Restart the Molecular Editor with multiple MSFs

Display the **Edit** menu and select the **Molecular Editor** function.

The Molecular Editor palette replaces the Molecular Modeling palette and the textport reads:

Only one MSF can be active in the editor at one time,
search1.msf will be kept active.

4. Change the active MSF.

In the Molecule Management Table select the **Active** cell for methanol.msf.

The **Active** cell in the search1.msf changes from **Yes** to **No**. The bonds of the methanol structure brighten while the bonds of the search1 structure are dimmed.

5. Move the methanol fragment.

Select **Move Fragment** from the Molecular Editor palette.

The message:

Pick atom in fragment to move
is displayed.

Pick any atom in the methanol structure.

The Fragment & Set Transformation Dials (Dial Set 2) are displayed.

Use translation dials to separate methanol from search1.

6. Convert methanol to methylhydroxyl.

Select **Add Atoms** from the Molecular Editor palette.

The Add Atoms palette is displayed and the Molecular Editor palette is removed.

Select **Convert to Hydroxyl** from the Add Atoms palette.

The message line reads:

Pick atom to convert

Pick a hydrogen in methanol. It is converted to a hydroxyl group.

Select **Exit Add Atoms**.

The Add Atoms palette is removed from the screen.

7. Select Save and Exit.

Select **Save and Exit** from the Molecule Editor palette.

A dialog box lists each of the open MSFs that can be saved.

Select **only methanol to be saved** and then select **OK**.

The 3D Molecular Editor Save Options dialog box displays the default options:

Reassign atom types

Reassign atom charges - Use Charge Templates

Rename Atoms Automatically During Exit

Select the default options by clicking the **OK** button.

In the Adjust Total Charge dialog box, select the option **All Atoms** then click **OK**.

In the Saving Options dialog box, select the option **Save to New File-name**.

In the File Librarian dialog box, enter the new name **methylhydroxal** in the filename entry field, and click the **Save** button.

The Molecule Management Table updates to a new name and new number of atoms.

Other editing options

The **Atom Property Editor** item in the **Edit** menu provides editing options, using a consistent interface, for atomic data functions contained in an MSF. This editor provides functions for editing residue and segment data as well as atomic data. It does not allow reordering of atoms or residues. The Atom Property Editor operates using a combination of the Property Editor palette, dialog boxes and the Atom and Residue tables.

[Table 15](#) lists the selections in the palette and provides a brief description of each.

The Atom Table is an editable table containing one row per atom. For multi-residue structures, this table does not appear by default. It can be generated by selecting **Atom Table** from the Property Editor palette or by double-clicking rows in the Residue Table. Only atoms that are currently displayed (visible) are listed in the table. For large structures, the table can display atoms, one residue at a time.

Table 16. Property Editor palette

Selection	Description
Atom Table	For single residue structures, toggles the display of the atom table. For multi-residue structures, creates an atom table containing information about all atoms.
Residue Table	Toggles the display of the residue table for multi-residue structures.
Coordinates from file...	Updates the atomic coordinates from an external dynamics, search, or general ASCII file.
Load Fourth...	Displays a scrolling list of extra information of types REAL, INT4, or ASTR (atom constraints) that can be loaded as current fourth parameter values.
Show Extra...	Lists the names of extra information stored within the MSF in the Textport.
Incorporate Extra...	Allows per-atom data contained in an external file to be included in an MSF as extra information. The data will automatically be loaded as the current fourth parameter.
Copy to Extra...	Allows internal data to be copied to extra information so that it can then be output to PDB/CRD files or used in labeling and coloring. The options include atomic charges, masses, and van der Waals radii.
Delete Extra...	Allows extra information to be deleted from the MSF.
Options...	Displays a dialog box containing options for the functionality of the editor.
Highlight Edit Residues	Toggles coloring of atoms available for editing. Available atoms are those listed in the Atoms Table. Default selection.
Save to MSF...	Causes current data in the displayed table to be saved to an MSF. Enabled when data in a table is edited.
Quit	Exits the Atom Property Editor without saving any changes to the tables.
Finish	Exits the Atom Property Editor saving all changes.

Table headings for the Atom Table are, from left to right:

- Row label – number of the atom in the MSF segment
- Segment name – read only
- Residue – residue ID (allows residues to be redefined)
- Name – atom name
- X coord – X coordinate
- Y coord – Y coordinate
- Z coord – Z coordinate
- Charge – atomic charge

2. Editing 3D Structures

- Type – atom type name
- Fourth – current fourth parameter or Bvalue (or Bvalue plus occupancy)

The table is automatically updated if the coordinates are changed using **Coordinates from File**, if residue centers are changed, or if a different fourth parameter is loaded. Altering data in the table automatically causes labels to be redrawn or a new conformation to be displayed.

The Residue Table is an editable table that is displayed when the structure to be edited contains more than one residue. If you double click with the mouse on a residue row or if you select **Atom Table** from the Property Editor palette, the Atom Table is also displayed. Double clicking a residue row when the Atom Table is displayed removes the atoms in the residue from the Atom Table.

Table headings for the Residue Table are, from left to right:

- Row label – number of the atom in the MSF segment.
- Seg – MSF segment name. Allows segment redefinition and renaming. Double clicking on the column header displays a dialog box for renaming each whole segment. Segments given the same name will be merged.
- ID – residue ID. Double-clicking the column header displays a dialog box for the automatic sequential number of residues within various segments.
- Name – residue name.
- Atoms – number of atoms in the residue. Read only.
- Cent X – the X coordinate of the residue centroid.
- Cent Y – the Y coordinate of the residue centroid.
- Cent Z – the Z coordinate of the residue centroid.
- Radius – maximum radius of the residue. Read only.
- MSF – MSF name. Read only.

The **Atom Data** selection in the **Edit** menu opens a pull-right menu that allows you to make changes in an atom charge, atom type, or other atom parameters such as hydrogen bonding or $E_{\min}$ values. The changes are made in dialog boxes that open when you make a selection from the pull-right menu.

The **Bond Options** selection in the **Edit** menu displays a dialog box where bond options are selected.

Summary

The Molecular Editor provides tools to construct and modify any 3D molecular structure. The application's basic editing capabilities provide ways for you to add or delete atoms, change atom types, build a structure by merging a number of molecular fragments, and prepare a structure for CHARMM operations. It assigns atom types and charges to all atoms and satisfies valence requirements by adding hydrogens to the structure during editing procedures.

Editing tools for this applications are located in the Molecular Editor palette that opens when you select **Molecular Editor** from the **Edit** menu in the menu bar.

Although you can build molecules from scratch, it is generally easier to begin construction in ChemNote, moving to the Molecular Editor when you have completed the basic structure.

Structures created with the Molecular Editor may not have accurate geometries. These geometries can be refined using an energy minimization process before you exit the Molecular Editor. The process is initiated by selecting **CHARMM Minimize** from the Molecular Editor palette.

In the Molecular Editor, a single MSF is created even if multiple fragments exist. You also may choose to create a CHARMM RTF for a single fragment. After the MSF and any optional RTFs are created, QUANTA returns to the Molecular Modeling application.

The Atom Property Editor provides editing options, using a consistent interface, for atomic data functions contained in an MSF. This editor provides functions for editing residue and segment data as well as atomic data. It does not allow reordering of atoms or residues. The Atom Property Editor operates using a combination of the Property Editor palette, dialog boxes, and the Atom and Residue tables.

The **Atom Data** selection in the **Edit** menu allows you to make changes in atom charge, atom type, or other atom parameters such as hydrogen bonding or $E_{\min}$ values.

The **Bond Options** selection in the **Edit** menu give you options for editing bonds.

2. Editing 3D Structures

3. Calculating and Minimizing Energy

This chapter covers potential energy and energy minimization calculations as they are executed in QUANTA using the CHARMM program. Read this chapter to understand basic information about CHARMM, the QUANTA-CHARMM interface, and how potential energy and energy minimization calculations are set up and completed.

For more detailed information about CHARMM, consult *CHARMM Principles* and the *CHARMM Dictionary*. For more information on forcefields and their uses, please see *Forcefield-Based Simulations*.

The exercises in this chapter use structures that were created in an earlier chapter. If you did not create and store the MSFs orange.msf and sodium.msf files, go through the exercises in Chapter 1 and do so. If you need to restart QUANTA, refer to the restart procedure in the Preface.

Understanding basic CHARMM operations

QUANTA uses the CHARMM program to execute many of the calculations needed for modeling. CHARMM is a general and flexible software application developed and maintained at Harvard University to model the structure and behavior of molecular systems. See the References at the end of this chapter for more information.

A variety of systems, from isolated small molecules to solvated complexes of large biological macromolecules, can be simulated using CHARMM.

CHARMM uses empirical energy functions to describe the forces on atoms in molecules. These functions, plus the parameters for the functions, constitute the CHARMM forcefield. CHARMM uses these functions to rapidly calculate conformational energies, local minima, barriers to rotation, energy surfaces, and time-dependent dynamic behavior.

The CHARMM energy functions

The CHARMM energy functions include internal coordinate terms and pairwise nonbond interaction terms. The total energy can be expressed by the equation:

3. Calculating and Minimizing Energy

$$\text{Energy} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{torsion}} + E_{\text{oop}} + E_{\text{elec}} + E_{\text{vdW}} + E_{\text{cons}} + E_{\text{user}} \quad \text{Eq. 1}$$

The internal energy terms include:

- Bond length (E_{bond})
- Bond angle (E_{angle})
- Torsion (dihedral) angle (E_{torsion})
- Out-of-plane (improper) torsion (E_{oop})

The external (i.e., nonbond) energy terms include:

- Electrostatic potential (E_{elec})
- van der Waals interactions (E_{vdW})

The extra energy terms include:

- Constraint energy (E_{cons})
- User-defined energy (E_{user})

The hydrogen-bond function is available but is not included by default in CHARMM calculations.

CHARMM theory

The standalone CHARMM 31b1 documentation can be found on the web here:

<http://www.accelrys.com/doc/life/charmm/31b1/doc/Charmm31.Html>

CHARMM calculations

CHARMM uses data from these three sources to calculate energies:

- Principle structure file (PSF)
- CHARMM parameters
- Cartesian coordinates for all atoms

The PSF identifies, by number and type, all atoms contained in the structure. Individual atomic masses and charges are included in this file. Additionally, the PSF lists all intramolecular parameters that contribute to the CHARMM energy function. These parameters include bonds, bond angles, torsion angles, and out-of-plane angles. A PSF is constructed from the data contained in an RTF and the CHARMM parameter file. For more information on PSFs and RTFs, see Chapter 1 of *QUANTA Basic Operations*.

The CHARMM parameter file defines force constants and reference geometries for each type of atom and interaction contained in structures. Cartesian coordinates are provided to CHARMM or are calculated by CHARMM from the standard geometry data contained in an RTF and the reference values stored in the CHARMM parameter file.

QUANTA interaction with CHARMM

QUANTA provides interactive access to CHARMM through a menu-driven graphical interface. QUANTA allows complex modeling problems to be solved by users with relatively little experience with CHARMM. In addition, QUANTA enables experienced CHARMM users to tap all of CHARMM's inherent flexibility.

Along with sending commands to CHARMM, QUANTA also sends the appropriate molecular definition and Cartesian coordinates required for the requested calculation. The molecular definition is contained in an RTF selected from the \$CHM_DATA directory, created by ChemNote or the Molecular Editor, or located in a PSF constructed by QUANTA. The Cartesian coordinates are contained in an MSF.

QUANTA provides an easy mechanism to set up, run, and monitor a variety of CHARMM calculations on structures. Some of these calculations, such as energy, minimization, and dynamics calculations, are explicitly called. These functions are selected from the Modeling palette that is displayed when QUANTA is in the Molecular Modeling mode. Other calculations are started automatically by QUANTA applications such as Sequence Builder.

calc and
min energy

3. Calculating and Minimizing Energy

The **CHARMm** menu, opened from the menu bar, controls both CHARMm access and calculation setup. Table 17 lists the menu items and provides a brief description of each.

Table 17. CHARMm menu functions

Selection	Description
Select CHARMmHost	Opens a pull-right menu with choices for interactive, batch, or NQS jobs. When a selection is made, the names of available CHARMm hosts are listed. The selected host is used for subsequent invocations of CHARMm. If no host is specified, QUANTA tries to run CHARMm locally.
Initialization Options	Opens a dialog box with a variety of initialization options, including the option to enter additional initialization commands.
CHARMm Process	Opens a pull-right menu that includes selections for starting, terminating, and reporting the status of interactive, batch, and NQS jobs. Does not detect the status of CHARMm jobs detached from QUANTA or started stand-alone.
Energy Terms	Allows the specification of energy terms to be included in the calculation. When possible, use all available energy terms.
Update Parameters	Allows the specification of parameters that control nonbond terms in CHARMm energy calculations.
Minimization Options	Allows the selection of a minimization technique and defines additional specifications that control the minimization calculation.
Dynamics Options	Allows the definition of specifications that control dynamic animation calculations.
Constraints Options	Opens a pull-right menu that allows the set up of constraints that cause CHARMm to fix or restrict the motion of atoms during minimization.
SHAKE Options	Allows the removal of very high-frequency vibrations from consideration in dynamics simulations.
Parameters	Opens a pull-right menu with Specify Files , Save Parameters , and Set Options Files selections. Choosing the Set Options selection opens a dialog box to select options on missing and relevant parameters and on report generation.
CHARMm Mode	Opens a pull-right menu with PSF , RTF , MMFF and MMFFS modes , PSF Terms , and RTF Options selections. The PSF Terms selection controls energy terms that are generated. The RTF Options selection controls the format of PSFs as well as the terms included in an RTF.
GetFourthParameter	Returns various per-atom scalar values or forces from CHARMm to MSF Extra Information so that the information is available for further display and calculation within QUANTA.
Periodic Boundaries	Allows entry of specific boundaries using shape matrix, lattice constants, or data from an MSF.
Optimize Hydrogens	Sends the HBUILD command to CHARMm for the current active structure.

Table 17. CHARMM menu functions (Continued)

Selection	Description
Solvate Structure	Allows selection of a solvent and image model for solvation. Initiates the process.
Send CHARMM Command	Allows sending of CHARMM command(s) to CHARMM from QUANTA. Initializes CHARMM if it is not already running.
Stream CHARMM File	Allows sending a command directly to CHARMM from QUANTA. Initializes CHARMM if it is not already running.
Capture Commands	Opens a pull-right menu with On , Off , Suspends , and Restart selections. Allows CHARMM commands sent from QUANTA to be captured in a script file and used again at a later time.
Settings	Opens a pull-right menu that includes Show Setup , Save Setup , and Restore Setup . Allows viewing of any portion of the current CHARMM setup, saving the setup, or replacing the current setup file with the contents of a saved setup file.

Results from CHARMM calculations are periodically sent back to QUANTA. Some results, such as energies, are displayed in the viewing area and in the textport. If new coordinates are calculated for a structure, these coordinates are incorporated into the MSF and the structure is redisplayed in the viewing area.

You have several options for saving MSF changes that result from CHARMM calculations or other structural modifications. These options are accessed through the dialog box that is displayed when **Save Changes** is selected in the Modeling palette. The Modeling palette is displayed whenever QUANTA is in Molecular Modeling mode. The options for saving changes are listed and described in Table 18.

calc and
min energy

Table 18. Save Changes Options dialog box

Option	Description
Create New Generation	Creates a new version of an MSF. This is the default action unless another default is specified within the Set MSF Savings Options selection in the Preferences menu.
Overwrite	Places the modified coordinates in the MSF by overwriting the current file. The previous conformation is lost.
Save to New Filename	Writes coordinates to a new file after a new base filename is entered in a dialog box.
Abort Saving to Disk	Retains coordinates in memory, but does not update the MSF on disk.

Generating a potential energy value

A CHARMM empirical energy calculation produces a potential energy value. A single-point energy calculation is useful in comparing conformations, computing thermodynamic properties, calculating interaction energies and forces, and evaluating structures during conformational searching. In addition to energy, CHARMM also calculates the forces on each atom in a molecular system.

When you request an energy calculation, CHARMM is automatically started from QUANTA. It remains running throughout the QUANTA session, accepting requests from QUANTA until it is explicitly stopped or the QUANTA session is ended.

Complete the following exercise to become familiar with the potential energy calculation process.

1. Visually set up orange.msf and sodium.msf for calculations.

In the **File** menu, select **Open** to display the File Librarian dialog box.

Select sodium.msf and orange.msf from the scrolling list of MSFs then select the **Replace** and **Open** buttons. The structures are displayed in the viewing area.

Select **Move Atom** from the Modeling palette. Pick the sodium ion and move it near the sulfide group of the organic sulfide molecule using the Translate dials on the Dial Emulator palette.

2. Save the coordinates for the new location of the sodium ion and display distance monitors.

Select **Save Changes** from the Modeling palette. In a dialog box that opens, select the option:

Create a new generation of sodium.msf

Select **Distance** from the Geometry palette. **Show Distance Monitors** is checked and highlighted in the palette by default.

Select the sodium ion and then select one of the three oxygen atoms on the organic sulfide molecule. Repeat this procedure two more times. You see a visual representation of the close ionic bonds that hold sodium and the rest of the molecule together.

Select **Distance** again to inactivate the selection.

3. Calculate the CHARMM potential energy.

Select **CHARMm Energy** from the Modeling palette. The tool is checked and highlighted.

CHARMm automatically starts and status information indicating the progress of the CHARMm calculation is displayed on the message line.

Additional status information, similar to the information listed below, is displayed in the textport.

```
RJRDMAN: server created
CHARMm changing to directory /usr/marj/accelrys_quanta
CHARMm job watsoncharmm22r2exe0 started on watson
UNIT 99 OPENED FOR READ ONLY ACCESS TO charmm.cis
INPUT STREAM SWITCHING TO UNIT 99
RDTITL> *.....
RDTITL> * CHARMm STARTUP FILE FOR QUANTA RDTITL *
CHARMm>! Redirect the CHARMm output
CHARMm> open write unit 7 Card name CHARMm.LOG line
UNIT 7 OPENED FOR WRITE ACCESS TO CHARMm.LOG
Line Buffering was set for I/O unit 7 if applicable.
CHARMm> outu 7
Using RTF as CHARMm data structure
```

4. Complete the CHARMm calculation.

When the calculation is complete, the potential energy is displayed in the upper-right corner of the viewing area. **CHARMm Energy** is no longer checked and highlighted on the Modeling palette.

A breakdown of the energy contributions similar to the text below is displayed in the textport. Your results will depend on the calculation parameters you chose and the position of the sodium ion.

The total CHARMm energy is: -32.8911

```
The individual contributions are as follows:
Bond energy      : 0.7448
Angle energy     : 25.7481
Dihedral energy  : 11.0324
Improper energy  : 7.3459
Lennard-Jones energy : 225131.1582
Electrostatic energy : -121.8766
Constraints, other : 0.0016
```

calc and
min energy

Performing a minimization

CHARMm minimization locates the molecular conformation with the lowest potential energy. Minimization is often used to prepare a structure for molecular dynamics.

CHARMm offers a choice of minimization techniques. With these choices, global minimum-energy conformations for small molecules or local minimum-energy conformations for larger molecular systems can be deter-

3. Calculating and Minimizing Energy

mined. You choose the best minimization technique for your structure. Table 19 lists the choices and describes each.

Table 19. Minimization techniques

Method	Description
Steepest Descents	A first-derivative method that improves a very poor conformation. Does not generally converge, but rapidly improves the conformation. The default method.
Conjugate Gradient	A first-derivative method that slowly converges to a local minimum. Suitable for molecular systems that start with reasonable conformations. Shows better convergence than steepest descents and allows larger coordinate shifts. Very poor conformations are more likely to fail than with steepest descents.
Powell Conjugate Gradient	A more efficient implementation of the conjugate gradient method. Does not provide an automatic facility to update the nonbond and hydrogen-bond interaction lists and is therefore recommended only in limited cases.
Newton-Raphson	Newton-Raphson minimization. Exhibits rapid convergence. Includes a facility for avoiding saddle points. Often requires excessive storage requirements or long computation time for large molecules. Restricted to molecular systems with 200 or fewer atoms.
Adopted Basis Newton-Raphson	Applies the Newton-Raphson algorithm to a subspace of the coordinate vector spanned by the displacement coordinates of the last positions. Similar to conjugate gradients, but results in fewer energy evaluations. Can be used to efficiently minimize very large molecular systems. No atom limitations in CHARMM.

When you run a minimization, define the minimization method and parameters first by choosing **Minimization Options** from the **CHARMm** menu in the menu bar. Table 20 lists the parameters you must define in the dialog box that is displayed when you select **Minimization Options**.

Table 20. Minimization Options dialog box

Parameter	Description
Number of Minimization Steps	If a tolerance is met before the maximum number of iterations, the calculation ends.
Coordinate Update Frequency	Number of minimization steps between each coordinate update from CHARMM to the QUANTA display and to the CHARMM log file.
Energy Gradient Tolerance	Tolerance applied to the energy gradient during each cycle of minimization. If the average gradient is less than the tolerance, the calculation ends.
Energy Value Tolerance	Tolerance applied to the differences between the energy values at each step during a cycle of minimization. If the energy difference is less than the tolerance, the calculation ends.
Initial Step Size	Initial step size for the minimization. For a detailed explanation, see <i>CHARMM Principles</i> . The default is 0.020.
Step Value Tolerance	If the step size is less than this tolerance, the calculation ends.

calc and
min energy

Run a minimization by selecting **CHARMM Minimization** from the Modeling palette. If CHARMM is not already running, it is automatically initialized when you select **CHARMM Minimization**.

The next exercise goes through the process of setting up and running a minimization calculation for the structures in orange.msf and sodium.msf.

1. With the structures displayed in the viewing area, select the minimization technique and parameters.

Display the **CHARMM** menu and select **Minimization Options**. A dialog box allows you to select a minimization method and specify associated parameters controlling the calculation.

Select the option:

Steepest Descents

Enter the values:

Number of Minimization Steps: 50

Coordinate Update Frequency: 5

Energy Gradient Tolerance: 0.00001

Energy Value Tolerance: 0.000

Initial Step Size: 0.020

Step Value Tolerance: 0.000

3. Calculating and Minimizing Energy

Select the **OK** button. The minimization technique and associated parameters are defined, and the dialog box is cleared from the screen.

2. Start the calculation.

From the Modeling palette, select **CHARMm Minimization**.

CHARMm automatically starts the minimization calculation, using the specified minimization technique and parameters.

Status information is printed in the message line indicating the progress of the CHARMm calculation. Additional status information is displayed in the Textport. **Undo Changes**, **Save Changes**, and **Reject Changes** are activated in the Modeling palette.

As the calculation proceeds, the coordinates representing a new conformation of the displayed structure are periodically sent back to QUANTA. The points at which these coordinates are sent to QUANTA is controlled by the **Coordinate Update Frequency** option in the Minimization Setup dialog box.

The structure is redisplayed with the new coordinates. In addition, the energy value calculated from these new coordinates is displayed in the upper right corner of the viewing area. The textport displays a minimization log similar to.

```
Minimization method: Steepest Descents    Total steps = 50

At step number 5  energy = -19.5813;  rms force = 7.349291
At step number 15 energy = -22.4063;  rms force = 7.018281
At step number 20 energy = -23.1046;  rms force = 6.854839
At step number 25 energy = -24.0076;  rms force = 2.107744
At step number 30 energy = -24.2339;  rms force = 7.462957
At step number 35 energy = -25.1297;  rms force = 2.279270
At step number 40 energy = -25.5521;  rms force = 1.715047
At step number 45 energy = -26.0209;  rms force = 3.248627
At step number 50 energy = -26.4346;  rms force = 2.168422
```

When the calculation is finished, the final conformation of the structure is displayed in the viewing area. The final energy is displayed in the viewing area and in the textport.

Performing repeated minimizations

If the requested **Energy Gradient Tolerance** or **Energy Value Tolerance** is not met before reaching the maximum number of minimization steps defined in the Minimization Setup dialog box, minimization calculations can be repeated. A repeat minimization calculation can use the same minimization method and parameters or a new method and new parameters.

Complete the following exercise to continue the minimization process for the structures in orange.msf and sodium.msf.

1. Select a new minimization technique.

Display the **CHARMm** menu and select **Minimization Options**. A dialog box allows you to select a minimization method and to specify associated parameters controlling the calculation.

Select the option:

Adopted-Basis Newton Raphson

Enter the values:

Number of Minimization Steps: 50
Coordinate Update Frequency: 5
Energy Gradient Tolerance: 0.0000
Energy Value Tolerance: 0.0001
Initial Step Size: 0.020
Step Value Tolerance: 0.000

Select the **OK** button. The minimization technique and associated parameters are defined, and the dialog box is cleared from the screen.

2. Start the second calculation.

From the Modeling palette, select **CHARMm Minimization**. CHARMm automatically starts the minimization calculation, using the specified minimization technique and parameters.

Status information is printed in the message line and textport.

As the calculation proceeds, the coordinates representing a new molecular conformation of the displayed structure are periodically sent back to QUANTA.

When the calculation is complete, the structure is redisplayed with new coordinates. In addition, the energy value calculated from these new coordinates is displayed in the upper right corner of the viewing area and in the textport.

calc and
min energy

Saving or rejecting calculation results

When a minimization calculation has produced an appropriate structure, the new coordinates of the minimized structure can be saved in an MSF by selecting **Save Changes** in the Modeling palette.

If you do not want to save minimized coordinates, select **Reject Changes** in the Modeling palette. When **Reject Changes** is selected, the minimized structure is replaced by the structure that was last saved to disk. All coor-

3. Calculating and Minimizing Energy

dinate changes, whether made by the minimization calculation or by any other calculation, such as **Move Fragment**, are lost.

The following exercise goes through the process of saving the structures in orange.msf and sodium.msf.

1. Save minimization results.

From the Modeling palette, select **Save Changes**.

A dialog box allows you to reject or save current changes for the file sodium.msf.

Select the option:

Save as a new generation of sodium.msf

Click **Save** to save the minimization results.

In the dialog box that opens for the orange structure, select the option:

Save as a new generation of orange.msf

Click **Save** to save the minimization results.

2. Rename and save the structures as a single MSF.

Display the **File** menu and select **Save As**. In the Write Options dialog box, select the following write options:

Write out current connectivity

Write out current bondtypes

Use the new MSF now

Select the **OK** button. In a File Librarian dialog box, enter the name orangeII and click **Save**. The new file orangeII.msf is displayed in the Molecule Management Table and the textport reads:

```
35 atoms selected for molecular structure orangeII.msf 35  
atoms will be displayed
```

The Merck Molecular Force Field

The Merck Molecular Force Field (MMFF), developed by Halgren at the Merck Research laboratories, is designed for use with a large variety of chemical systems. Its pivotal application is the study of receptor–ligand interactions involving proteins or nucleic acids as receptors and a wide range of chemical structures as ligands. The forcefield can describe ligand and receptor in isolation as well as bound.

MMFF is a computationally derived energy expression that can accurately be applied to condensed-phase and aqueous processes. It uses a unique functional form for describing van der Waals interactions and employs novel combination rules that systematically correlate van der Waals parameters with those that describe experimentally characterized interactions involving rare-gas atoms. The MMFF energy expression is:

$$E_{\text{MMFF}} = \sum E_{B_{ij}} + \sum E_{A_{ijk}} + \sum E_{BA_{ijk}} + \sum E_{OOP_{ijk;l}} + \sum E_{T_{ijkl}} + \sum E_{vdw_{ij}} + \sum E_{Q_{ij}} \quad \text{Eq. 2}$$

where:

$E_{B_{ij}}$ bond stretching

$E_{A_{ijk}}$ angle bending

$E_{BA_{ijk}}$ stretch–bend interactions

$E_{OOP_{ijk;l}}$ out-of-plane bending at tri-coordinate centers

$E_{T_{ijkl}}$ torsion interactions

$E_{vdw_{ij}}$ van der Waals interactions

$E_{Q_{ij}}$ electrostatic interactions

Constituent terms of the energy expression are calculated in kcal/mol. They are described in detail elsewhere.^{2,3}

To allow straightforward application to condensed-phase simulations employing explicit solvent molecules, MMFF uses a dielectric constant in its electrostatic interaction terms.

To apply the MMFF

1. Select **CHARMm mode** from the **CHARMm** menu.
2. Select **MMFF** from the **CHARMm mode** pull-right menu. A textport message reads:

Subsequent CHARMm calculations will use MMFF mode.

The task is now complete.

calc and
min energy

Summary

This chapter describes the basis and procedures for running potential energy and energy minimization calculations. These calculations are exe-

3. Calculating and Minimizing Energy

cuted in QUANTA using the CHARMM program created and maintained by Harvard University.

QUANTA provides interactive access to CHARMM through a menu-driven graphical interface. When you request an energy calculation in QUANTA, CHARMM is automatically started and remains running until it is explicitly stopped or the QUANTA session is ended.

Energy functions plus parameters for the functions constitute the CHARMM forcefield. Much of QUANTA's modeling analysis is based on the CHARMM forcefield.

CHARMM uses data from three sources to calculate energies: a principle structure file (PSF), CHARMM parameters, and Cartesian coordinates for all atoms. A CHARMM empirical energy calculation produces a single potential energy value.

Sequential potential energies and their rate of change are the basis of energy minimization. CHARMM minimization locates the molecular conformation with the lowest potential energy. You may select one or any combination of five methods used in CHARMM for a minimization calculation. The results of a calculation may be accepted and saved or rejected

References

1. B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan, M. Karplus "CHARMM: A program for macromolecular energy, minimization, and dynamics calculations", *J. Comp. Chem.* **4** 187–217.
2. Halgren, T. A., *J. Amer. Chem. Soc.* **114** 7827–7843 (1992).
3. Halgren, T. A., *The Merck Molecular Force Field*, privately published paper available from Accelrys.
4. *Forcefield-Based Simulations*, Accelrys, San Diego.

4. Building with Sequence Builder

This chapter describes the basics of using the QUANTA Sequence Builder application. Read this chapter to learn procedures for building and editing sequences for proteins, nucleic acids, and other polymers

In Sequence Builder, you can construct residue sequence lists for proteins, amino acids, and polymers using predefined residue libraries and structure fragments. The application can also read existing sequence files.

After a sequence is defined, it is automatically sent to CHARMM where Cartesian coordinates are constructed using CHARMM internal coordinate information. The graphical representation of the structure is then displayed in Molecular Modeling mode.

An RTF describes the molecular topology of each residue in a sequence and contains the information necessary to compute the energy of a structure as well as perform other calculations. Atom names, types, masses, and partial atomic charges are included in an RTF. Coordinates are not included.

Patch residues modify atoms after a sequence is assembled. These patches describe a deviation from the standard residue definition. For example, the RTF for cysteine generates a single cysteine residue, but does not contain information for linking two cysteine residues together via a disulfide bond. The disulfide bond is specified by applying the patch residue DISU to each of the two cysteines. A disulfide bond can also be applied to form linkages between segments.

Patches can be applied to any residue, and a residue can have more than one patch. Selecting a patch name from the palette automatically inserts the patch at the insertion point.

When a sequence of residues is specified, a secondary conformation can be applied, using conformations provided by QUANTA. Sequences can also have user-defined conformations.

The basic steps in creating a structure with the Sequence Builder are:

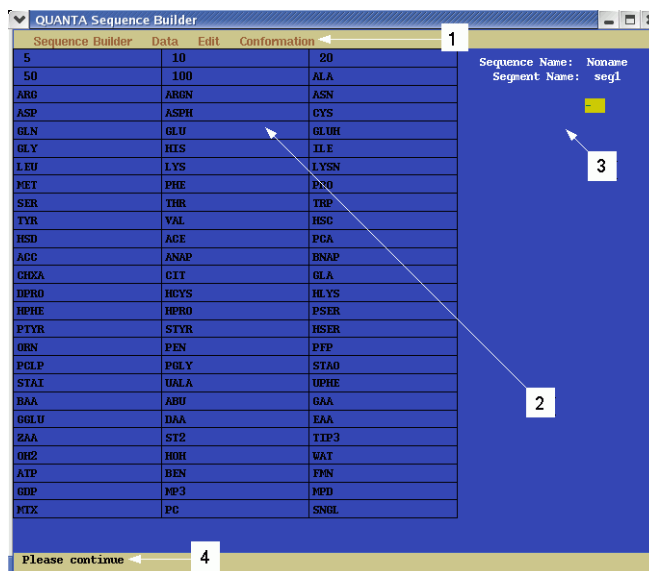
- Select a set of residue topology files.
- Define the sequence.
- Apply patches as required
- Apply secondary conformations as required.
- Exit Sequence Builder, sending the sequence definitions to CHARMM for minimization.

4. Building with Sequence Builder

Sequence Builder is started from the within Molecular Modeling. To start Sequence Builder, open the pull-right **Builders** menu in the **Applications** menu and select **Sequence Builder**. Once Sequence Builder is started, all work in Molecular Modeling is suspended until Sequence Builder is exited.

Understanding the Sequence Builder window

The Sequence Builder application displays a new window over the other QUANTA windows. This window can be resized, moved, iconified, pushed, and popped in the same manner as all other standard workstation windows.



The Sequence Builder window is made up of four distinct areas. Although some window areas are the same as other QUANTA applications, the menu bar and palette are specifically customized for Sequence Builder.

1. Menu bar

The menu bar contains four menu items: **Sequence Builder**, **Data**, **Edit**, and **Conformation**. **Sequence Builder** menus are displayed as pull-down or sticky menus. [Table 21](#) lists these selections and provides a brief description of each.

Table 21. Sequence Builder menus

Selection	Description
Sequence Builder	Provides information about the application and returns QUANTA to the Molecular Modeling application.
Data	Reads previously created sequence files into the Sequence Builder. Saves newly generated residue sequences. Deletes and renames sequences.
Edit	Modifies a residue sequence using operations such as delete, copy, and move. Items in a sequence are selected by marking residues or sets of residues.
Conformation	Includes functions for applying secondary conformations to a residue sequence and examining the values of residue dihedral angles.

Tables 22 through 24 list the selections in the menus under the entries of the menu bar.

2. Palette

Residues available in a selected RTF are displayed in the palette. Palette selections also include repeat numbers to specify multiple residues of the same type and residue specifications based on single-letter amino acid codes.

3. Viewing area

The viewing area is used as a notepad to list residue names in sequence from left to right. The beginning of each line contains an integer designating the residue number of the first residue in that line. The name of the current sequence and segment are displayed at the top of the viewing area.

4. Message line

The message line provides information about current operations or directions about how to proceed.

building
seq viewer

Table 22. Sequence Builder menu

Selection	Description
About the Sequence Builder	Provides general information about the Sequence Builder application.
Return To Molecular Modeling	Exits from the Sequence Builder application and returns to the Molecular Modeling application.

Table 23. Data menu

Selection	Description
Read Sequence File	Prompts for the name of a sequence file. Reading a sequence file overwrites any sequence currently displayed in the viewing area.
Read PDB File	Reads a Protein Data Bank (PDB) file and overwrites any sequence currently displayed in the viewing area.
Append Residues/ Patches to Palette	Displays the File Librarian, listing RTFs in the current directory. Selecting an RTF adds the residues and patches defined in the RTF to the palette for a broader selection.
Rename Sequence	Prompts for a new name for the sequence being defined. The new name is displayed above the current sequence.
Rename Segment	Prompts for a segment selection and a new name, which is then displayed at the top of the selected segment.
Delete Sequence and Restart	Clears the current sequence from the viewing area. Any work not previously saved is lost.
Create New Segment	Prompts for a new segment name. The name appears below the last line in the sequence.
Load New Segment From File	Creates a new segment by reading a sequence from a file.
Write Segment File	Saves a marked segment to a specified file. The current sequence remains unchanged.
Write Sequence File	Saves the current sequence in a specified file. The sequence remains in the viewing area after it is saved.
Write CHARMM File	Creates a CHARMM command input file to build the CHARMM PSF for this sequence. This file is automatically generated when exiting Sequence Builder and saving the sequence.
Write Hydrophobic- ity File	Creates a file of X, Y data, representing the residue number versus the residue hydrophobicity. The data can later be viewed with Graphs in the Molecular Modeling File menu. Hydrophobicity information is available only for proteins.

Starting Sequence Builder

When you open Sequence Builder, the application displays a new window over other QUANTA windows. The window can be manipulated in the same manner as other windows in QUANTA. The Sequence Builder is started from Molecular Modeling. When Sequence Builder is running, all work in Molecular Modeling is suspended.

Sequence Builder is accessed from the **Applications** menu opened from the menu bar in QUANTA. Select **Builders** from the **Applications** menu. Then select **Sequence Builder** from the **Builders** pull-right menu.

Table 24. Edit menu

Selection	Description
Add Residues To Sequence	Displays a palette that contains the available residues. A number of identical residues are added consecutively to the sequence by selecting a repeat number followed by the residue name. Residues are always inserted at the current insertion point.
Apply Patches to Residues	Displays a palette that contains the available patches. Patches are applied by first selecting a patch from the palette, then marking residues where the patch is to be applied. Patch atoms are compared to the atoms of the marked residue for validation. If atoms are missing, the patch is not applied to the residue.
Link Polysaccharide Monomers	Creates linkage points for polysaccharide monomers. The file POLYSACH.RTF does not contain linkage points. Therefore, when polysaccharide monomers are added to the viewing area, they are not linked together.
Unmark Items	Removes marks from all residues, patches, or segments in the sequence.
Move Marked Item	Moves marked residues to the insertion point. The insertion point may not be defined within a marked residue range.
Copy Marked Item	Copies marked residues to the current insertion point. The marked residues remain in their current position. The insertion point may not be within the marked residue range.
Copy Item n Times	Prompts for the number of times to duplicate marked residues, then copies the marked residues at the current insertion point the designated number of times. The marked residues remain in their current position. The insertion point may not be defined within a marked residue range.
Delete Marked Item	Deletes all marked residues, patches, and segments.
Scroll Up	Moves the viewing area up 26 lines. This is useful when there are more residues in the sequence than can be displayed in the viewing area.
Scroll Down	Moves the viewing area down 26 lines. This is useful when there are more residues in the sequence than can be displayed in the viewing area.

Sequence Builder is initialized by reading a CHARMm RTF containing the building blocks from which a sequence is constructed. RTF definition files are distributed in the directory \$CHM_DATA and are accessed via the File Librarian. A File Librarian dialog box is opened whenever Sequence Builder is started.

See Appendix D of *QUANTA Basic Operations* for tables identifying the residues and patch residues contained in the RTF definition files.

Table 25. Conformation Menu

Selection	Description
Set Secondary Conformation	Provides a secondary conformation for a protein sequence. The palette changes, giving the instruction to mark a residue or residue range and to designate where the folding will take place. A scrolling list dialog box displays a list of the secondary conformations to choose from.
Examine and/or Edit Torsions	Displays the values of dihedral angles and allows them to be modified by directly specifying new dihedral angles. The palette tools change to provide prompts for selecting residues. After each residue selection, a dialog box displays the current value of the dihedral. Entering a new value changes the residue's conformation. Phi, psi, and omega angles can be changed.
Highlight Torsional Changes	Indicates which residues have had conformational changes by highlighting their residue names.

Building a sequence

When you start Sequence Builder, an insertion point appears in the viewing area as a highlighted dash. Residues are added to the sequence before the insertion point, thus keeping the insertion point at the end of the sequence. You can move the insertion point to a location preceding any residue. After the insertion point is moved, selected residues are added to the sequence at this new location rather than at the end of the sequence.

A sequence is comprised of one or more residues. Residues are grouped together into segments. You can add a single residue to a sequence by selecting the residue name from the palette. Several residues of the same type can be added by selecting a repeat number from the palette prior to selecting the residue name.

Patch residues modify atoms after a sequence is assembled. These patches describe a deviation from the standard residue definition. For example, patches can modify N- and C- terminal groups or form disulfide bridges within or between segments.

When a patch that links two residues is applied, the residues are counted as residues 1 and 2 in the opposite order of their selection.

Complete the following exercises to open Sequence Builder and become familiar with basic building techniques.

1. Open Sequence Builder.

Display the Applications menu and select **Builders**. Open the pull-right menu and select Sequence Builder from the pull-right menu. The Sequence Builder window, containing a File Librarian dialog box, is displayed over the QUANTA windows.

2. Select a residue definition file.

From the File Librarian dialog box scrolling list, select AMINO.RTF and then click **Open**. The File Librarian is removed from the screen and residues contained in AMINO.RTF are displayed in the palette.

3. Construct a sequence.

Select the repeat number **10** from the palette and the message line prompts:

Pick the residue you want repeated.

Select the residue ALA from the palette. Ten ALA (alanine) residues are displayed in the viewing area with a hyphen before each residue. The insertion point is positioned immediately after the tenth residue. A number appears at the beginning of each line designating the residue number of the first residue on that line.

4. Add 100 residues to the end of the sequence.

Select the repeat number 100 on the palette and then select the residue ARG.

One hundred ARG residues are added to the end of the 10 ALA residues.

5. Mark the first 10 residues in the sequence.

Move the cursor over the first ALA residue in this sequence and click the left mouse button. The residue is highlighted, indicating it is marked.

Move the cursor over the last ALA residue in this sequence and click the left mouse button again. All 10 ALA residues are now highlighted, indicating they are all selected. The insertion point, however, remains at the end of the entire sequence of ALA and ARG residues.

6. Add a copy of the first 10 residues to the end of the sequence.

Display the **Edit** menu and select **Copy Marked Item**. The 10 ALA residues are copied and inserted at the end of the sequence before the

4. Building with Sequence Builder

insertion point. The sequence now consists of 10 ALA - 100 ARG - 10 ALA.

7. Unmark the ALA residues.

Display the **Edit** menu and select **Unmark Items**. The 10 ALA residues are no longer highlighted, indicating they are no longer marked.

8. Insert 100 residues before the ARG residues.

Move the cursor to the dash before the first ARG residue and click the left mouse button. The insertion point moves to this location.

Select the repeat number 100 and then select the residue GLU. One hundred GLU residues are added between the ALA and ARG residues. The insertion point is still located before the first ARG residue. The sequence now consists of 10 ALA - 100 GLU - 100 ARG - 10 ALA.

9. Scroll through the entire sequence.

Display the **Edit** menu and select **Scroll Down**. The last section of the sequence is now displayed in the viewing area and the first section is no longer displayed.

Redisplay the **Edit** menu and select **Scroll Up**. The first section of the sequence is again displayed in the viewing area.

10. Delete residues.

Mark the first 10 residues in the sequence. Then display the **Edit** menu and select **Delete Marked Item**. The 10 ALA residues are removed from the sequence.

The sequence now consists of 100 GLU - 100 ARG - 10 ALA. The insertion point is still located before the first ARG residue.

11. Delete the remainder of the sequence.

Display the **Data** menu and select **Delete Sequence and Restart**. A dialog box is displayed, requesting a name for the new sequence.

Enter **peptide** in the dialog box and click the **OK** button. Another dialog box warns that the currently displayed residue will be deleted.

Click the **Yes** button, indicating the current sequence is to be deleted, and the dialog box is removed from the screen. The old sequence is removed, and the new sequence name peptide is displayed at the top of the viewing area.

Creating a peptide

In *QUANTA Basic Operations*, the small peptide molecule, PEPTIDE.msf, was displayed. This section builds this molecule with Sequence Builder just as the original structure was built.

The Sequence Builder provides common secondary conformations that can be applied to residue sequences. The application also provides the option to assign specific dihedral angles to selected residues.

Available secondary conformations include:

- Extended Backbone (180.0°)
- Right-Handed Alpha Helix
- Left-Handed Alpha Helix
- Antiparallel Beta Sheet
- Parallel Beta Sheet
- Modified Beta Sheet
- Proline 1
- Proline 2
- C 7 Equilateral
- C 7 Axial
- Beta Turn Type I (-,-,-,0)
- Beta Turn Type I' (+,+,+,0)
- Beta Turn Type II (-,+,+,0)
- Beta Turn Type II' (+,-,-,0)

When you save a sequence to a file, the file extension .seq is automatically appended to the base filename. When you exit Sequence Builder, the information in the .seq file is used to create a CHARMM command input file (*filename.STR*). This file is automatically created and submitted to CHARMM, where the Cartesian coordinates are built. These coordinates are then returned to the Molecular Modeling application for display and inclusion in an MSF.

Complete the following exercise to build, modify, and save a peptide to an MSF.

1. Enter residues in the new sequence.

4. Building with Sequence Builder

In the listed order, select each of the following 20 residues to create the sequence. As each residue is selected, it is displayed in the viewing area.

ALA, PHE, VAL, LEU, THR, SER, ASP, TYR, SER, LYS, TYR, LEU, ASP, SER, ARG, LYS, ILE, VAL, LEU, ALA

2. Apply secondary conformation.

Display the **Conformation** menu and select **Set Secondary Conformation**. The list of residues in the palette is replaced by the instructions:

Pick residue or range of residues.

Mark the first four residues, ALA, PHE, VAL, and LEU, in the sequence and click the **OK** button. In a dialog box containing a scrolling list of the secondary conformation options, select the option:

Extended Backbone (180.0)

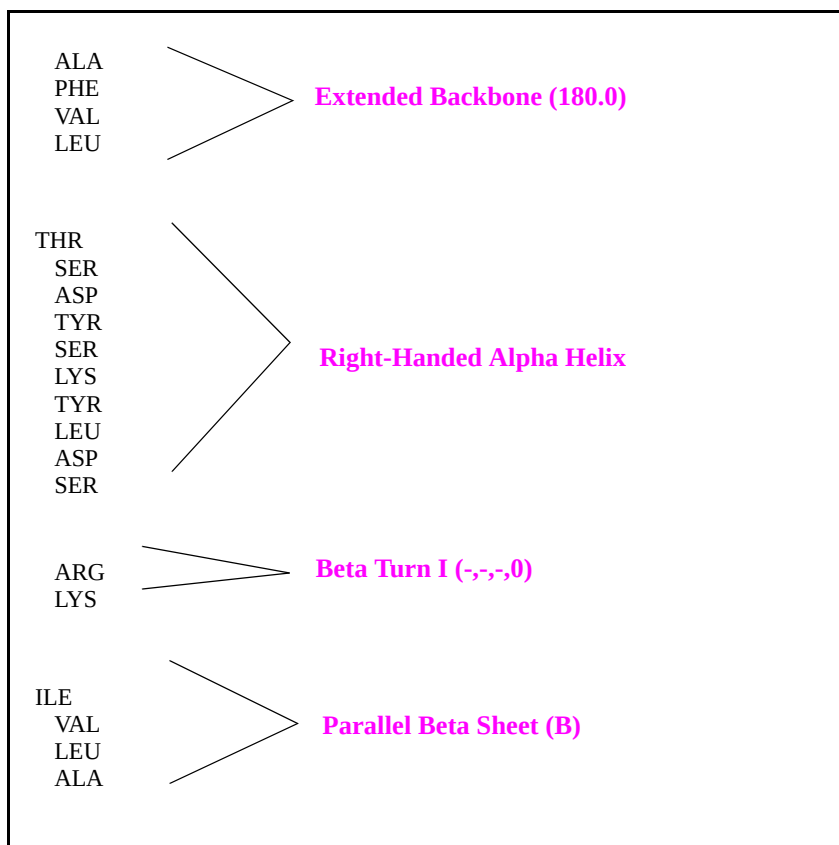
Select the **OK** button. The dialog box is removed from the screen, the secondary conformation is applied to the marked residues, and the marks are removed from the residues.

3. Select additional secondary conformations for the rest of the peptide.

Consulting [Figure 1.](#), mark each remaining group of residues and select the indicated secondary conformation. When you have assigned all sec-

ondary conformations, click the **Done** button in the palette. The secondary conformation palette is replaced with a list of residues.

Figure 1. . Secondary conformation for peptide



4. Create an MSF from the sequence.

Display the **Sequence Builder** menu and select **Return to Molecular Modeling**. Since the peptide structure has not been saved, a dialog box asks if the changes are to be saved. Click the **YES** button and the message line reads:

Validating links between residues.

Sequence Builder checks to make sure that residues are properly assembled and patches applied appropriately.

The File Librarian is displayed. Enter mypeptide in the **Filename** data entry field and select the **Save** button. The File Librarian and the Sequence Builder window are removed from the screen, revealing the

4. Building with Sequence Builder

Molecular Modeling window. QUANTA automatically starts a CHARMM command input file to build the Cartesian coordinates for the sequence.

Minimizing a peptide

Structures created in Sequence Builder have approximate geometries (bond lengths and bond angles). These geometries need to be refined through a minimization process before continuing with other modeling operations.

Complete the following exercise to minimize the structure in mypeptide.msf.

1. Display mypeptide in the Molecular Modeling window.

When the creation of mypeptide.msf is complete, a dialog box allows the structure that was just created to be used.

Select the option:

Use the new molecule mypeptide.msf only

then click the **OK** button. The structure mypeptide is displayed in the Molecular Modeling viewing area.

2. Minimize the peptide.

Display the **CHARMM** menu and select the **Minimization Options** function. In a dialog box that contains the minimization setup options, select the option:

Adopted-Basis Newton Raphson

Enter the values:

Number of Minimization Steps: 50

Coordinate Update Frequency: 5

Energy Gradient Tolerance: 0.000

Energy Value Tolerance: 0.000

Initial Step Size: 0.020

Step Value Tolerance: 0.000

Click the **OK** button and the dialog box is cleared from the screen and new minimization parameters are established.

From the Modeling palette, select **CHARMM Minimization** to start the CHARMM calculation. The cursor changes from an arrow to a

watch and the message line displays information regarding progress of the minimization process.

Minimization is completed when the cursor is restored to an arrow. The final conformation of the structure is displayed in the viewing area. The minimized energy results are displayed in the upper-right corner of the viewing area and in the Textport.

3. Save minimization results.

From the Modeling palette, select **Save Changes** and a dialog box enables the new coordinates of mypeptide.msf to be saved.

Select the option:

Create New Generation of mypeptide.msf

Click the **OK** button. The dialog box is cleared from the screen, the textport indicates that the old structure file is renamed mypeptide.msf,001, and the minimized structure is saved in mypeptide.msf.

Creating a cyclic peptide

You also can build cyclic peptides in Sequence Builder using the same residue and patch libraries used for linear peptides. Complete the following exercise to construct the cyclic peptide, CCK7. This peptide will be used in a search exercise in Chapter 4 of *QUANTA Simulation and Analysis*.

4. Start Sequence Builder.

Display the **Applications** menu. Select **Builders** and then select **Sequence Builder** from the pull-right menu that is displayed. The Sequence Builder window and a File Librarian dialog box are displayed over the QUANTA window.

From the scrolling list in the dialog box, select the file AMINO.RTF and then click the **Open** button. The File Librarian is removed from the screen, and the residues contained in AMINO.RTF are displayed in the Sequence Builder palette.

5. Enter the residues in the sequence.

Select the following residues (in the order shown) to create a peptide sequence:

4. Building with Sequence Builder

TYR
MET
GLY
TRP
MET
ASP
PHE

As each residue is selected, it is displayed in the viewing area.

6. Set Secondary Conformation.

Display the **Conformation** menu and select **Set Secondary Conformation**. The list of residues in the palette is replaced by the instructions:

Pick residue or range of residues

and by the **OK**, **Done**, and **Unmark** buttons.

Mark the GLY and TRP residues and click the **OK** button in the palette. In a dialog box containing a scrolling list of available secondary conformations, select the scrolling list entry:

Beta Turn 1 (-,-,-,0)

Click the **OK** button. The dialog box is removed from the screen and the conformation is applied to the two residues.

Click the **Done** button in the palette. The Secondary Conformation palette is replaced by a list of residues, along with the Sequence Builder window.

7. Apply Patches.

Display the **Edit** menu and select **Apply Patches to Residues**. The patches contained in AMINO.RTF are displayed in the palette replacing the display of residues.

8. Apply a patch to the sequence.

Select the LINK patch from the palette and the message line reads:

Please select 2 residues to apply patch to.

Mark TRY, the first residue in the sequence, and the residue is highlighted.

Mark PHE, the last residue in the sequence, and the sequence changes to indicate the link between the residues.

9. Return to Modeling and save the peptide.

From the Sequence Builder menu, select **Return to Molecular Modeling**. In a dialog box that offers the option to save the changes, click the **YES** button.

In a File Librarian dialog box, enter the name:

CCK7

Click the **Save** button. The File Librarian and the Sequence Builder window are removed from the screen revealing the Modeling window. QUANTA automatically starts CHARMM to build Cartesian coordinates for the sequence. A dialog box asks if the just created structure is the structure to use.

Select the option:

Use the new molecule CCK7.msf only

Select the **OK** button and the structure CCK7.msf is displayed as a cyclic structure. The link patch imposes a covalent bond between the N alpha and C-terminal atoms. The cyclic conformation is created during minimization, when the lowest energy value is calculated for this bond.

10. Set up minimization for CCK7.msf.

Display the **CHARMM** menu and select **Minimization Options**. In a dialog box containing the minimization setup options, select the option:

Adopted-Basis Newton Raphson

Enter the values:

Number of Minimization Steps: 200

Coordinate Update Frequency: 5

Energy Gradient Tolerance: 0.0100000

Energy Value Tolerance: 0.000000

Initial Step Size: 0.020000

Step Value Tolerance: 0.000000

Select the **OK** button and the dialog box is cleared from the screen.

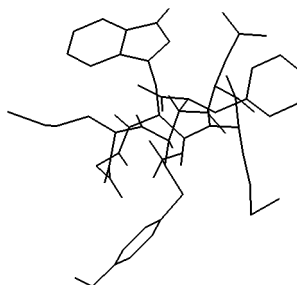
11. Run a minimization for CCK7.msf.

Display the Modeling palette and select **CHARMM Minimization** to start the CHARMM calculation.

When minimization is completed, the final conformation of the structure is displayed in the viewing area. The minimized energy results are displayed in the upper-right corner of the viewing area and reported in the textport. The cyclic conformation is created as a result of calculating

4. Building with Sequence Builder

the lowest energy value of the covalent bond between the N alpha and C terminal atoms.



12. Save minimization results.

Display the Modeling palette and select **Save Changes**.

In a dialog box that offers the opportunity to save the new coordinates of CCK7.msf, select the option:

Overwrite CCK7.msf

Select the **OK** button and the dialog box is cleared from the screen.

Summary

Sequence Builder is used to construct residue sequence lists for proteins and polymers using predefined residue libraries and structure fragments. Sequence Builder also can read and edit previously created sequence files. After a sequence is defined, it is automatically sent to CHARMM, where Cartesian coordinates are constructed using CHARMM internal coordinate information. Using patch residues, cyclic peptides and other modifications can be applied to linear structures.

The basic steps in creating a structure with Sequence Builder are:

1. Select a set of residue topology files.
2. Define the sequence.
3. Apply patches as required.
4. Apply secondary conformations as required.

5. Exit Sequence Builder, sending the sequence definitions to CHARMM for coordinate construction and minimization.

When a structural build is complete, the molecule is ready to use in other QUANTA operations.

4. Building with Sequence Builder

5. Using Other Build Applications

This chapter describes building and modeling applications accessed through the **Applications** menu. These applications extend the capabilities of QUANTA for particular types or forms of molecules or for particular approaches to modeling. The applications include:

- Crystal Modeling.
- Solvent/Amorphous Builder.
- Protein applications.
- X-ray applications.
- De novo design applications.
- NMR Structure Determination.

All these applications are supplied as optional packages with core QUANTA.

Read this chapter or portions of it to become familiar with how to access and use any of these applications. Additional documentation is available for optional applications. See the preface for a complete list of QUANTA and QUANTA-related documentation.

Using Crystal Modeling

Crystal Modeling provides tools to generate and modify a system based on translational periodicity or crystallographic symmetry. Crystal Modeling can interactively build periodic or crystalline structures from:

- Proteins.
- Polymer segments.
- Biopolymer segments.
- Small molecules.
- Other QUANTA molecules.

Crystallographic spacegroups can be used to create symmetry-related copies of the original molecule. The appropriate symmetry information can be sent to CHARMm.

5. Using Other Build Applications

Crystal Modeling operates in two modes: real atom mode and symmetry atom mode. In real atom mode, symmetry copies extend the size of the structure by creating new atoms. The size of a system generated in real atom mode is subject to the normal QUANTA atom limits.

In symmetry atom mode, symmetry copies exist only as abstract data. No physical atoms are created. Any changes to the asymmetric unit are immediately reflected in the symmetry copies. Symmetry atoms are displayed as graphical objects and cannot be picked or manipulated as real atoms can.

Symmetry information can be saved to an atom selection file, *filename.asd*, and used subsequently in Crystal Modeling to generate symmetry copies. Symmetry information can also be sent to CHARMM to obtain a correct energy computation for the crystal. Once CHARMM is provided with symmetry information, subsequent energy minimization and dynamics operations also use symmetry images in their calculations. Crystal Modeling additionally provides a tool to perform lattice optimization in CHARMM, where CHARMM minimization modifies the unit cell parameters as well as the atom positions to optimize the crystal structure.

The atoms selected in QUANTA just before entering Crystal Modeling are used as the template from which symmetry-related copies are built. Although a structure might have its own internal symmetry, this atomic system is referred to as the asymmetric unit. If CHARMM calculations are to be performed on the crystal, the asymmetric unit must be an MSF.

When you exit Crystal Modeling, symmetry copies can be retained or discarded. When they are retained, additional modeling, including minimization, dynamics, and conformational searches, can be carried out on the molecular structure in the crystalline environment. However, all symmetry copies should be removed before attempting to reenter Crystal Modeling to correctly calculate CHARMM images.

Defining and incorporating symmetry information

As you enter the Crystal Modeling application, it detects whether the MSF contains symmetry information. If there is no symmetry information in the current MSF, a dialog box displays a list of spacegroups available in the symmetry library file \$HYD_LIB/symlib.sym.

This file lists symmetry operators that generate all equivalent positions in a unit cell for each of the standard spacegroups. The list of available space groups can be expanded to include nonstandard settings by editing the symmetry library file and adding the appropriate information.

When the MSF contains symmetry information, an opportunity to use this information or select another space group is offered. If symmetry information stored in the current MSF is not used, a new MSF is created to store

the specified symmetry information with the molecular structure. A dialog box is displayed offering MSF saving options.

The initial unit cell dimensions (a , b , c , α , β , γ) must be specified. Enter only the dimensions that can be defined independently for a given spacegroup. If spacegroup C2 is selected, for example, a dialog box is displayed to enter the unit cell dimensions a , b , c , and β .

In some cases, you are also prompted to define a unique axis by providing an orthogonalization method code. Orthogonalization codes determine the orientation of the unit cell axis and its reciprocal (abc and $a^*b^*c^*$, respectively), with respect to the xyz modeling axis. The orthogonalization code is usually set to 1. Table 26 lists the codes and their definitions.

Table 26. Orthogonalization codes

Code	Code description
1	a is parallel to x , c^* is parallel to z (Brookhaven default)
2	b is parallel to x , a^* is parallel to z
3	c is parallel to x , b^* is parallel to z .
4	hex $a+b$ parallel to x , c^* is parallel to z (Gerard Bricogne/ trigonal space groups)
5	a^* is parallel to x , c is parallel to z (FRODO default)

Crystal Modeling allows the asymmetric unit to be modified while symmetry copies exist. Symmetry copies are updated to reflect modifications in the asymmetric unit. When **Modify Asymmetric Unit** is selected, a palette is presented to provide a specific set of selections for this function.

Using the Crystal Modeling palette

The Crystal Modeling palette provides selections for interactively generating a crystal by creating symmetry copies, displaying the unit cell, and changing the unit cell dimensions. The palette also provides access to CHARMM for calculating the energy of the crystal structure and creating symmetry images. Table 27 lists the palette selections and provides a brief description of each.

Calculating CHARMM energy using images

CHARMM makes symmetry copies of a primary molecule or collection of molecules by creating a set of images. Each image is given a unique name and a set of instructions. These instructions are in the form of matrices describing the rotation and translation needed to generate the image.

Table 27. Crystal Modeling palette

Selection	Description
Show Unit Cell	Generates and displays the edges of the unit cell, which is helpful in visualizing placement of the symmetry copies. Show Legend must already be selected. The dimensions of the unit cell are displayed in the upper-right corner of the viewing area.
Show Legend	Displays a legend containing structural information in the lower-right corner of the viewing area.
Modify Cell Parameters...	Adjusts cell parameters, including cell size.
Define Symmetry...	Displays a series of dialog boxes to define or edit the space group, dimensions of the crystal cell, and orthogonalization code.
List Copies	In the textport, displays a list of operators and translations for symmetry copies.
Modify Symmetry Copies...	Opens a palette that allows you to add and delete copies and to create symmetry copies within an LMN box of user-defined dimensions.
Modify Asymmetric Unit...	Modifies the conformation and orientation of the asymmetric unit while retaining the crystal symmetry. The coordinates of the asymmetric unit are modified by a rotation, translation, or torsion angle adjustment. Then each symmetry copy is created by taking the new coordinates and applying the symmetry data. The symmetry copies are updated and redrawn as the asymmetric unit is modified.
Normalize Unit Cell	Moves all atoms to positions within the unit cell.
Modify Fractional Coordinates	Displays a table that list all atoms and their coordinates. Coordinates may be edited in the table.
Surfaces...	Displays a palette from which planes of the crystal can be defined and displayed.
Display/Use Symmetry Bonds	Displays and allows manipulation of symmetry bonds.
CHARMm Energy/Image	Creates a CHARMm image file and sends it to CHARMm to calculate the energy of the crystal structure.
Minimize Crystal	Minimizes the crystal using CHARMm. The energy reported when all atoms are physically present includes an intramolecular energy term for each symmetry copy and all pairwise interactions between copies falling within the prescribed nonbond cutoff. When image data is in effect, only the intramolecular energy term for the asymmetric unit is calculated, in addition to all interactions between the asymmetric unit and image atoms falling within the cutoff.
Save	Saves minimized crystal information to an MSF.

Table 27. Crystal Modeling palette (Continued)

Selection	Description
Reject	Rejects the crystal structure that is displayed. Returns to the original structure.
Powder Diffraction	Displays the Powder Diffraction palette with selections for executing a powder diffraction and calculating and plotting the results.
Write to File	Saves symmetry information in the format of symmetry selection commands and writes to an atom selection definition file, <i>filename.asd</i> . The commands in the file can be read in subsequent sessions to re-create the symmetry copies.
Read From File	Reads symmetry information from an atom selection definition file, <i>filename.asd</i> , and displays symmetry copies as graphical objects. Symmetry copies defined in the file can be included in the viewing area with existing copies or can be displayed alone.
Exit from Crystal Builder	Exits Crystal Modeling and returns to Molecular Modeling. Symmetry copies can be retained as graphical objects or discarded.

The **CHARMm Energy/Image** selection creates a CHARMm image file and sends it to CHARMm with a request for the energy of the crystal structure. This file includes the coordinates of the asymmetric unit and the image commands needed to generate a crystal identical to the one displayed in the viewing area.

Update Parameters in the **CHARMm** menu is used in this calculation and should be set prior to starting Crystal Modeling. Appropriate values for **Image Update Frequency** and **Image Cutoff Distance** are specified in the Update Parameters dialog box.

The energy computed when images are in effect includes the intra-molecular energy of the asymmetric unit alone, plus the interaction energy between the asymmetric unit and image atoms falling within the image cutoff, each interaction being evaluated only once.

If the cell constants or other parameters defining the crystal are subsequently changed, the CHARMm image file is also updated. The modified image file is used in subsequent selections of **CHARMm Energy/Image**.

After the selection is used, you can exit Crystal Modeling and perform more extensive CHARMm calculations on the displayed crystal in the Molecular Modeling application. All modeling operations including minimization, dynamics, and conformational search can be performed with the CHARMm images in effect, preserving the specified crystal symmetry.

During energy minimization or molecular dynamics, the atoms of the asymmetric unit and the symmetry copies are displayed in the viewing area. However, only coordinates for the atoms of the asymmetric unit are written to the dynamics trajectory files. Despite the fact that all atoms are not

5. Using Other Build Applications

explicitly present, the energies reported are those of the molecular structure in the defined crystalline environment.

CHARMm energies for a collection of real atoms differ from those obtained using image data. The energy reported when all atoms are physically present includes an intra-molecular energy term for each of the symmetry copies and all pairwise interactions between copies falling within the prescribed nonbond cutoff.

When image data is in effect, only the intramolecular energy term for the asymmetric unit is calculated, in addition to all interactions between the asymmetric unit and image atoms falling within the cutoff range.

Nevertheless, reliable conformational modifications, such as minimizations, can be performed using energies obtained with CHARMm images.

In subsequent QUANTA sessions, the image file created in Crystal Modeling can be sent to CHARMm. This is accomplished by renaming the image file (charmm.img) to charmm_img.str, so that it is recognized as a stream file. The **Stream CHARMm File** selection in the **CHARMm** menu can then send the file to CHARMm. These image files function correctly only when the original asymmetric unit is displayed in the viewing area.

Modifying the asymmetric unit

The **Modify Asymmetric Unit** selection provides a way to modify the asymmetric unit in Crystal Modeling while retaining the crystal symmetry. When you make this selection, the Modify Asymmetric Unit palette opens over the Crystal Modeling palette. Selections on this palette are listed in [Table 28](#). A torsion template file must be selected prior to modeling the asymmetric unit. When you select **Read Torsion Template** from the Model Asymmetric Unit palette, a File Librarian allows you to select the file that defines adjustable torsions. Torsions that are part of a ring system or cyclic structure should not be defined in a torsion template file.

The Model Asymmetric Unit palette contains selections for rotating and translating the entire molecular structure or changing specific torsions. If you select **Rotate Atoms** or **Translate Atoms**, a palette opens over the Model Asymmetric Unit palette. These palettes contain adjustable torsions displayed as selections.

The **Rotate** and **Translate** selections cause a transformation of the asymmetric unit to occur. The unit of change is degrees when **Rotate** is active and angstroms when **Translate** is selected.

In the following exercise, Crystal Modeling procedures define a space-group, specify unit cell dimensions and orthogonalization code, specify lattice translations, display symmetry copies, and incorporate symmetry

Table 28. Modify Asymmetric Unit palette

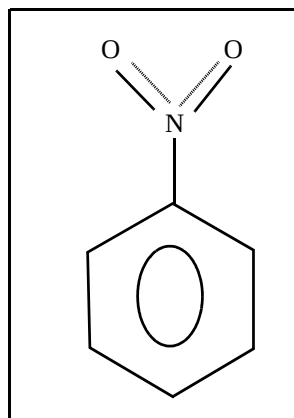
Selection	Description
Modify Torsions	Modifies the named torsion angle.
Translate Atoms	Opens a palette for translating the asymmetric unit along the z axis.
Rotate Atoms	Opens a palette for rotating the asymmetric unit about the z axis.
Read Torsion Template	Opens a dialog box with a list of torsion template files.
Select Atoms	Opens palette for selecting portions of the molecule and modifying the display of the structure.
Update Image	Updates image information for the symmetric unit display to incorporate asymmetric unit changes.
Exit Modify Asymmetric Unit	Exits Modify Asymmetric Unit and returns to Crystal Modeling.

information into an MSF. For this exercise, build the structure nitrobenzene in ChemNote. If you have not completed Chapter 1 on 2D structure sketching, do so before you continue with this exercise.

1. Create a structure to use in generating a crystal.

Display the **Applications** menu and select **Builders**. From the pull-right menu, select **2D Sketcher**. The ChemNote window is displayed.

Sketch the structure nitrobenzene.



2. Return to Molecule Modeling mode with the structure.

Display the ChemNote **File** menu and select **Return to Molecule Modeling**. A dialog box asks if the changes should be saved.

Select **Yes** and the File Librarian dialog box is displayed.

Enter the text nitrobenzene and click **Save**. A dialog box is displayed offers several options for adjusting partial charges.

Enter the value:

The desired net charge is: 0.000

Select the option:

CT, CH1E, CH2E, CH3E, C5R, C6R, C5RE, C6RE, HA types

Click the **OK** button.

The ChemNote window is removed from the screen, revealing the Molecular Modeling window. When the conversion of nitrobenzene.mol to nitrobenzene.msf is complete, a dialog box offers options for displaying MSFs.

Select the option:

Use the new molecule nitrobenzene.msf only

Click the **OK** button, and the nitrobenzene structure is displayed in the viewing area.

3. Setup energy minimization for nitrobenzene.msf.

Structures created in ChemNote frequently need to be optimized using energy minimization before modeling operations are started.

Display the **CHARMm** menu and select **Minimization Options**. In a dialog box containing the minimization setup options, select the option:

Adopted-Basis Newton Raphson

Enter the values:

Number of Minimization Steps: 100

Coordinate Update Frequency: 5

Energy Gradient Tolerance: 0.001

Energy Value Tolerance: 0.000

Initial Step Size: 0.020

Step Value Tolerance: 0.000

Click the **OK** button. The dialog box is cleared from the screen and new minimization parameters are established.

4. Start minimization for nitrobenzene.msf.

From the Modeling palette, select **CHARMm Minimization**. As the CHARMm calculation begins, the cursor changes from an arrow to a watch. The message line displays information regarding the progress of the minimization process, which is completed when the watch is restored to an arrow.

The minimized energy results are displayed in the upper-right corner of the viewing area and in the textport.

5. Save the minimization results.

In the Modeling palette, select **Save Changes**. A dialog box offers the option to save the new coordinates of nitrobenzene.msf.

Select the option:

Create New Generation of nitrobenzene.msf

Select the **OK** button and the dialog box is cleared from the screen. The textport indicates that the old structure file is renamed nitrobenzene.msf,001 and the minimized structure is saved in nitrobenzene.msf.

6. Start the Crystal Modeling application.

Display the **Applications** menu and select **Crystal Modeling**. From the scrolling list in the Space Group dialog box, select the option:

P1 #1 triclinic

Click the **OK** button.

In the Enter Dimensions for Triclinic Cell dialog box, enter the values:

a: 10
b: 10
c: 10
alpha: 90
beta: 90
gamma: 90

Click the **OK** button and the Enter Orthogonalization Code dialog box is displayed.

Accept the default value:

Integer Value: 1

Click the **OK** button and the Crystal Modeling palette is displayed.

5. Using Other Build Applications

7. Modify Symmetry Copies.

From the Crystal Modeling palette, select **Modify Symmetry Copies** and the Symmetry Copies palette is displayed.

Select **Add LxMxN Box**. In the Enter Box Dimensions dialog box, enter the values:

	from	to
l	-1	1
m	-1	1
n	-1	1

Click the **OK** button. The 26 symmetry copies are created and displayed in the cubic volume.

Click the **Reset View** button in the Dial Emulator palette and apply global rotations so that all copies can be seen.

From the Symmetry Copies palette, select **Exit Symmetry Copies** and the palette is removed from the screen.

8. Select Symmetry mode.

From the Crystal Modeling palette, select **Symmetry Mode**. Each symmetry copy is converted from structures with real atoms to images that are graphical objects. The **Minimize Crystal** selection is also enabled.

9. Select Minimize Crystal.

From the Crystal Modeling palette, select **Minimize Crystal**. The lattice parameters are optimized along with the molecule in the crystal environment. **Save** and **Reject** are enabled.

From the palette, select **Save** and the new coordinates are saved in nitrobenzene.msf

10. Exit Crystal Builder.

From the Crystal Modeling palette, select **Exit Crystal Builder**. A dialog box asks if copies are to be retained.

Select the option:

Delete copies

Click the **OK** button. The copies are deleted and the Modeling palette is redisplayed.

Using protein applications

The QUANTA **Applications** menu contains optional protein applications:

- Protein Design.
- Protein MODELER.
- Protein Health.
- Protein Profile Analysis.

Protein Design is an application for manipulating and analyzing protein structures. It uses and extends the molecular graphics capabilities of QUANTA and its interface to CHARMM for proteins.

Protein MODELER is an automated protein homology package that builds a 3D model for a protein sequence using data from the alignment of the sequence with one or more homologous proteins.

Protein Design includes tools for predicting secondary and tertiary structure, alignment, superimposition, homology, and protein modeling. It can only be accessed from the **Application** menu and activates two palettes, Protein Design and Protein Utilities.

The Protein Health application provides tools for qualitative analysis of protein structures. With this application, you may examine the quality of structural parameters, such as backbone and sidechain conformation and overall molecular packing, to visually determine nonstandard areas or conditions in the molecule.

Protein Health is packaged with Protein Design or may be used in combination with the X-ray or NMR applications. It can be accessed from the **Applications** menu or from within Protein Design.

The Protein Profile Analysis application characterizes the environment around each residue in a protein structure to generate a protein profile. The profile, composed of a matrix of characteristics, can be used to compare protein structures globally and locally and to evaluate the quality of a generated homology model.

Protein Profile Analysis can be accessed from the Applications menu or from within Protein Design.

Documentation of the protein applications is available in the *Protein User's Guide* and the *Protein Reference*.

Using X-ray applications

The X-ray applications X-AUTOFIT, X-BUILD, X-POWERFIT, X-LIGAND and X-SOLVE provide tools for building the 3D coordinates of proteins and nucleic acids into electron density. The interfaces to CNX and X-PLOR facilitate structure refinement.

The X-AUTOFIT application provides tools to trace C α coordinates into electron density as part of the de novo process of X-ray structure determination. The application provides semi-automated tools to build C α atoms using “bones” skeletonization of the electron density. Sequence assignment using fuzzy logic and three automated methods to convert the C α trace into all-atom models are provided.

The X-POWERFIT application provides automated methods for tracing C α coordinates into electron density maps and represents a rapid method for map interpretation.

X-BUILD provides tools for building all-atom models into electron density. These include three types of real-space torsion angle refinement (rigid-body refinement, loop fitting, and regularization) and several manual tools for model building.

X-LIGAND is an application for the automated fitting of complex ligands into omit/difference electron densities, including conformational searching of flexible ligands.

X-SOLVE provides an automated method for water fitting into electron density.

The interfaces to CNX and X-PLOR allow refinement of crystal structures using both crystallographic data and intramolecular and crystal interactions.

Documentation of the X-ray applications is available in *X-Ray Structure Analysis*.

Using NMR Structure Determination

The NMR Structure Determination application provides tools to build and refine 3D molecular models from NMR data. This application features an interactive link between spectrum and structure. It also features interfaces to CNX and X-PLOR for structure calculation and refinement, including distance geometry, simulated annealing, restrained molecular dynamics, energy minimization, NOESY back calculation, and relaxation matrix anal-

ysis. NMR Structure Determination provides a complete set of graphical and statistical tools for evaluation of the quality of structures.

Summary

Crystal Modeling generates and modifies structures based on translational periodicity or crystallographic symmetry. The applications can build periodic or crystalline structures from proteins, polymer segments, biopolymer segments, and small molecules. Symmetry information can be sent to CHARMM, and additional investigations can be performed in other QUANTA applications.

The Protein applications are used to manipulate, analyze, and evaluate protein structures. They may be used together or individually with other building and refining applications.

The X-ray applications provide tools to build and refine 3D molecular models from X-ray crystallographic data.

The NMR Structure Determination application provides tools to build and refine 3D molecular models from NMR data.

5. Using Other Build Applications

6. Using Graphical Objects

This chapter describes the graphical representation of calculations in the QUANTA Molecular Modeling application. Read this chapter if you plan to use graphical objects to visualize structural data. The objects covered in this chapter include:

- Ribbons.
- Grid contour meshes for displaying atom surfaces determined by van der Waals radii.
- 3D vector displays.
- Displaying Quanta plot files.
- Color scale.
- Connolly solvent surfaces.
- Brick maps from probe and molecule interaction energy field maps.
- Electrostatic potential energy surfaces (2D and 3D).
- Electrostatic fields.

In addition, the chapter includes a section on generating and displaying hydrogen bonds.

Graphical objects are displayed in relation to, but separate from, the structures on which they are based. Although each object is a representation of data related to a structure, it is not part of the MSF. However, the option, **Attach to MSF** in the Object Creation dialog box is checked as a default selection. This option allows you to attach an object to an MSF so that it may be moved and deleted with the structure. Using the **Attached** column of the Object Management Table, you may toggle the object/MSF attachment. The Object Management Table also provides object display, naming, and deletion options. Each graphical object is uniquely identified so that you can manage it throughout a QUANTA session.

Some objects such as ribbons, Connolly solvent surfaces, and grid contour meshes are generated within QUANTA. Other objects such as brick maps and 3D vectors are generated from results of calculations outside of QUANTA.

Generating ribbons

Ribbons are graphical objects that trace peptides, protein backbones, or any other molecular chain through guide atoms that occur in all residues of a molecular structure. The ribbon-drawing algorithm used in QUANTA is from methods cited in references 1 and 2 in the Reference section of this chapter.

In QUANTA, the alpha carbon and carbonyl oxygen atoms of each protein residue act as default guide atoms for drawing a ribbon. Guide atoms occur in all residues. The ribbon is offset 1.2 Å from the alpha carbon position. Ribbon defaults are set to optimally display alpha helices in proteins.

Guide atoms, ribbon width, number of threads, and ribbon color can be changed through the **Draw** menu by accessing the pull-right menu **Object Parameters** and selecting **Ribbon Parameters**. A dialog box enables you can make changes.

Complete the next exercise to become familiar with the procedure for generating and manipulating a ribbon. To complete this exercise, you need to use the MSF mypeptide.msf. This file was created as part of an exercise in the section *Creating a Peptide* in Chapter 4. Complete that exercise before you proceed.

1. Display the structure.

Display the **File** menu and select **Open**. In the Open MSF File Librarian dialog box, select mypeptide.msf from the scrolling list.

Click the **Replace** button and then the **Open** button. The structure contained in the file mypeptide.msf is displayed in the viewing area.

2. Create a ribbon.

Display the **Draw** menu and select **Create Objects**. A dialog box offers options for creating several graphical objects.

Select **Ribbon Structure** and then enter **ribbon** and **8** in the respective **Object Name** and **Object Color** data entry fields.

Accept the default option, **Attach to MSF**. The name of the open MSF, mypeptide.msf, is displayed in the box next to this selection. The ribbon is attached to this MSF and can be moved and deleted with the MSF.

Click the **OK** button.

The dialog box is closed, and a ribbon consisting of six strands is drawn through the C α and O atoms in the backbone of mypeptide.msf.

The four middle strands are displayed using color 8. The two outside threads are a different color, providing a 3D representation of the backbone chain.

The Object Management Table opens over the Molecule Management Table, displaying the name and status of the ribbon.

Generating a grid contour mesh

Grid contour meshes are graphical objects that provide an efficient and visually effective method of displaying surfaces on atoms. All active atoms or a selection of atoms may be used in generating the grid. Atom surfaces are determined by the van der Waals radii of the current atom selection. Selected atoms are defined in the context of other atoms in the structure.

When a grid contour mesh is created about a methyl group attached to a phenyl ring, you may include or exclude the atoms in the phenyl ring. Including the atoms in the ring creates a grid that is open at the point where the methyl group is attached to the phenyl ring. If the atoms in the ring are excluded, an enclosed grid is created.

1. Create a grid contour mesh for all atoms.

Display the **Draw** menu and select **Create Objects**. In the dialog box for creating objects, select the option **Grid Contour Mesh**. Then enter **grid1** and **4** in the **Object Name** and **Default Object Color** data entry fields, respectively.

Select the option **Attach to MSF** and the name of the open MSF, mypeptide.msf, is displayed in the box next to the option.

Click the **OK** button and a dialog box offers options for the selecting atoms to define the grid.

Accept the default text **all** by clicking the **OK** button. A dialog box appears with options that select atoms to define the context of the grid.

Accept the default text **all** by clicking the **OK** button. The dialog box is cleared from the window, and a grid contour mesh is displayed around the structure mypeptide.msf in color 4.

Two graphical objects are now displayed with the structure mypeptide.msf: the ribbon and the grid contour mesh. The Object Management Table lists both objects.

Turn off the display of both objects by selecting the top cell in the **Displayed** column. Both objects are removed from the screen, and the entry

6. Using Graphical Objects

for each in the **Displayed** column of the Object Management Table changes from yes to no.

2. Create a Grid Contour Mesh from Selected Atoms.

Display the **Draw** menu and select **Create Objects**. A dialog box offers options for creating several graphical objects.

Select the option **Grid Contour Mesh**, then enter **grid2** and **14** in the **Object Name** and **Object Color** data entry fields, respectively.

Select **Attach to MSF** and the name of the open MSF, mypeptide.msf, is displayed next to the option.

Click the **Interactive** button and the Atom Selection Utilities and Select Atoms palettes are displayed.

From the Select Atoms palette, select **Include** and **Pick Atom**.

In the viewing area, pick any three atoms in different areas of mypeptide.msf, and the ID for each selected atom is displayed. The three picked atoms define the center of each portion of the grid contour mesh.

From the Select Atoms palette, select **Finish** and the palettes are removed from the screen. A dialog box offers options for selecting atoms to define the context of the grid.

Enter the text **All** and click the **OK** button. The grid contour meshes are displayed around the selected atoms in the viewing area and the Object Management Table lists the object GRID2 and its status.

3D vector displays

If your structure has 3D vector information, you can display a vector for each atom. The information is stored as fourth parameter information of type REA3 in the .msf.

Vector data representing forces can be transferred from CHARMM to the .msf using **Get Fourth Parameter** in the CHARMM menu and selecting **Forces** from the pull-right menu. This extra information is labeled FORCE.

Vector data from external sources can be imported into a .msf by selecting **Incorporate Data** from the **Edit** menu, selecting **Vectors** from the pull-right menu, and specifying a file from the list in the File Librarian that is displayed.

To display 3D vectors

1. Select **Create Objects** from the **Draw** menu, select **3D Vectors** in the dialog box that is displayed, then click **OK**. A dialog box is displayed

prompting you to enter the label under which the vector data is stored. A list of labels and their types is output in the textport.

2. Enter a label of type REA3, then click **OK**. A new dialog box is displayed.
3. Select the options you want to use for your vector display. The linear scaling factor may need trial-and-error adjustment depending on the magnitude of the vectors to be represented. By default, the color of a vector is related to its magnitude and the colors are scaled from number 7 to 14.
4. When you have selected the options you want in this dialog box, click **OK**. Vectors are displayed as arrows attached to atoms on your structure.

The task is now complete.

QUANTA plot files

You can generate a QUANTA plot file (.qpt) to move graphical information to or from another application, to generate hardcopy images, or for other purposes. When a .qpt file is available, you can display the graphical information in it by creating a QUANTA plot file object. This display mechanism is an alternative to using **Plot Molecules/Preview** in the **File** menu.

To display a QUANTA plot file

1. Select **Create Objects** from the **Draw** menu, choose **QUANTA Plot File** in the dialog box that is displayed, then click **OK**. A File Librarian is displayed.
2. Select the .qpt file that you want to display, then click **OK**. A dialog box is displayed.
3. Select one of the two display options for the extent of display that you want, then click **OK**. The 2D image is displayed in the model window. You may have to scale this window to see a complete view of the structure.

Color scale

In the lower left corner of the molecule window, you can display a scale that shows the current color values. You also may add a maximum and minimum value to this display to indicate the value range to which these colors apply. Typically, this scale is used in conjunction with work where you have colored the structure according to some property, such as atomic charge.

6. Using Graphical Objects

To generate a color scale

1. Select **Create Objects** from the **Draw** menu, choose **Color Scale** in the dialog box that is displayed, then click **OK**. A dialog box is displayed.
2. In the dialog box, indicate the range of color numbers, toggle **Annotate Scale** on or off and, if you are annotating the scale, supply minimum and maximum values, then click **OK**. A color scale is displayed in the molecule window.

The task is now complete.

Managing objects

The Object Management Table is the primary means for managing objects. Each graphical object is uniquely identified so that you can manage it throughout a QUANTA session. The Object Management Table lists:

- Name of current objects
- MSFs with which the objects are associated
- Display status of each object
- Deletion status of each object
- Attachment status of each object and its associated structure

Each object is manipulated with a set of toggles that are activated by selecting the appropriate cell in the Object Management Table. The table functions in a manner similar to the Molecule Management Table. For example, you can mask the display of grid1 generated in a previous section by selecting the cell in the **Displayed** column of the Object Management Table that corresponds to grid1. When you make this selection, the cell information changes from **yes** to **no** and the grid is removed from the viewing area.

Complete this exercise to become familiar with the Object Management Table.

1. Display all objects.

The Object Management Table lists three objects: RIBBON, GRID1, and GRID2.

Select the **Displayed** cells for RIBBON and GRID1. All three objects are displayed, and each **Displayed** cell reads **yes**.

2. Mask the display of one object.

Select the **Displayed** cell again for grid1. The cell information changes from **yes** to **no** and grid1 is removed from the viewing area. The ribbon and grid2 remain displayed.

3. Detach an object from its associated MSF.

Select the **Attached** cell for grid2. The cell information changes from **yes** to **no**. No change is observed in the viewing area.

Go to the **File** menu and select **Open**. In the Open MSF File Librarian dialog box, select PEPTIDE.msf from the scrolling list. Then select the **Replace** option and click the **Open** button. The mypeptide structure is replaced by the PEPTIDE structure and the RIBBON and GRID1 objects are deleted. Grid2 remains displayed and listed in the Object Management Table.

4. Attach an object to an MSF.

Select the **Attached** cell for GRID2. The cell information changes from **no** to **yes**, and the file name PEPTIDE.msf appears in the MSF column.

5. Change the name of the object.

Select the **Name** cell for GRID2 and a dialog box offers the option to rename the object.

Enter **TESTGRID** in the name field and click the **OK** button. The name in the Object Management Table changes from GRID2 to TESTGRID.

6. Close the MSF and delete the remaining object.

Go to the **File** menu and select **Close**. When the dialog box opens, select **Close All** then **OK**. The peptide structure is removed from the viewing area and the object is deleted.

Solvent surfaces

Connolly solvent surfaces are graphical objects that are used to study the shape, depth, and chemical characteristics of receptor sites in a molecular structure. These surfaces provide effective representations of such important atomic and molecular properties as surface-solvent accessibility and electrostatic potential.

In the **Calculate** menu, the **Solvent Surfaces** selection provides an interface to an external program that calculates Connolly surfaces by rolling a

6. Using Graphical Objects

probe sphere over the surface of a molecular structure. See citation 3 in the References section of this chapter.

Calculations can be run on hosts other than the local system. To do this, display the **Calculate** menu and select **Select Host**. In the dialog box that opens, select a host. Then proceed with the calculation by returning to the **Calculate** menu and selecting **Solvent Surfaces**.

Calculation results are written to a surface file, filename.srf, and a solvent surface is displayed as a graphical object. You can have the map be displayed automatically on completing the calculation or at a later time by selecting **Create Objects** from the **Draw** menu.

Complete the following exercise to become familiar with the process of creating a Connolly surface. The exercise uses the structure, nitrobenzene created in the Crystal Modeling section of Chapter 5. If you have not completed the first part of the exercise in this chapter, do so before you proceed.

1. Open nitrobenzene.msf.

Open nitrobenzene.msf and display the structure in the viewing area.

2. Start a Connolly solvent surface calculation.

Display the **Calculate** menu and select **Solvent Surfaces**. From the pull-right menu that opens, select **Calculate**. A dialog box provides surface options. See Table 29 for a list of the options and a brief description of each.

Select the option:

Wait for Calculation to Complete

Enter the values:

Probe Radius: 1.4

Dot Density: 20.0

Select the options:

Solvent Accessible Surface

Use Active Atoms

These selections specify the type and display of the surface and the atomic context for the calculation.

Click the **OK** button and the Select Atoms and Selection Utilities palettes open.

From the Select Atoms palette, select **Include** and **All Atoms**, and then select **Finish**.

3. Name the Surface file.

In a File Librarian dialog box, enter the name:

nitrobenzene

Click the **Save** button and the filename extension .srf is automatically entered in the data entry field. The calculation starts and the cursor changes to a watch while the calculation is in process.

4. Display the Connolly solvent surface as a graphical object.

When the calculation of the surface is complete, a dialog box offers the opportunity to enter a name for the surface object.

Enter the name:

Connolly1

Click the **OK** button and a dialog box opens with options for selecting the atoms to be surfaced and the color of the surface.

Select the options:

All Atoms

Use Atom Colors

Display Big Dots

Click the **OK** button and the surface is displayed over all atoms, using the atom colors. The Object Management Table lists Connolly1 and its status.

5. Delete the surface object.

In the **Object Management Table**, toggle the **Delete** cell of the Connolly1 object listing from **no** to **yes**. The surface is deleted from the viewing area. However, the file nitrobenzene.srf is not deleted.

6. Re-create the surface object.

Once a surface file has been created, the surface object can be displayed at any time.

Display the **Draw** menu and select **Create Objects**. In the dialog box that opens, select:

Solvent Surface Maps

Attach to MSF

Enter the object name:

Connolly2

Accept the default color and click the **OK** button. In the File Librarian dialog box that opens, select nitrobenzene.srf from the scrolling list and then click the **Open** button.

A dialog box opens for entering information on a variety of object display parameters. See Table 30 for a list of options and a brief description of each.

Select the options:

All Atoms

Single Color

Display Plus Symbols

Enter the text:

Color Number: 14

Click the **OK** button. The surface is displayed and the Object Management Table opens listing the Connolly2 object.

7. Delete the graphical object.

Repeat the process used for Connolly1.

In the Object Management Table, toggle the **Delete** cell of the Connolly2 object listing from **no** to **yes**. The surface is deleted from the viewing area. However, the file nitrobenzene.srf is not deleted.

Table 29. Solvent surface options

Option	Description
Wait for Calculation to Complete	Runs the surface program as a foreground process. No modeling operations are performed until the surface is calculated.
Don't Wait; Run in Background	Runs the surface program in the background. Modeling tasks can be performed while the surface is being calculated, and the job status can be checked using Show Status in the Calculate menu. Solvent Surfaces in the Draw menu displays the surface when the calculation ends
Don't Run; Save Input Files.	Creates the input files for later use. Does not run a calculation.
Probe Radius	Specifies the diameter of the probe sphere. This value determines the surface sampling rate. The default value for the probe radius is 1.4 Å, which is the approximate size of a water molecule.
Dot Density	Specifies the number of dots per square angstrom (dots/Å). The default is 20.0 per angstrom. This value produces a useful surface in a reasonable time (for small molecules).

Table 29. Solvent surface options (Continued)

Option	Description
Type of surface	
Molecular Surface Calculation	Calculates the surface traced out by the edge of the probe of a particular radius.
Electrostatic Potential Surface	Uses partial atomic charge values to calculate an electrostatic potential molecular surface x.
Solvent Accessible Surface	Calculates the surface traced out by the center of the probe sphere as it rolls over the surface.
Calculate Buried Surface Only	Calculates a surface point generated when the probe's van der Waals radius overlaps with atoms in another structure. This is the surface at the interface between two molecules, inaccessible to the probe spheres. This option is only available when two MSFs are active.
Atoms forming context of calculation	
Use Active Atoms	Considers the currently selected atoms for the surface. This produces an accurate surface if all atoms are included in the selection. If the surface is confined to a specified area, an inaccurate surface may be generated.
Use All Atoms from Current MSFs	Considers the contribution of all atoms in the current molecular structures when the surface is calculated. This option calculates the surface for an entire structure.

Table 30. Surface display options

Option	Description
Display surface for which atoms?	
All Atoms	Uses all information in the surface file to display the surface. The surface surrounding all atoms selected when the surface was calculated is displayed as a graphical object.
Selected Atoms Only	Displays the surface for the current atom selection. The surface may have been calculated for an entire molecular structure, but if the atoms are not currently selected, the corresponding surface is not displayed.
Coloring options	
Use Atom Colors	Uses the current color selection information to color the surface the same color as the atoms associated with it.
Color On Energy	Colors each surface point according to the surface energy, used in conjunction with the electrostatic potential surface. The maximum and minimum energies and a range of colors are shown in a series of dialog boxes. These values can be accepted or re-specified. By default, a smooth range of colors is assigned to color numbers 7–14.
Single Color	Assigns a single color to the entire surface.

Table 30. Surface display options (Continued)

Option	Description
Color Number	Assigns a color number for the single color option.
Dot Symbol	
Display Little Dots	Surface display uses small dots.
Display Big Dots	Surface display uses big dots.
Display Plus Symbols	Surface display uses plus symbols.
User-Defined Symbol	Surface display uses user-defined symbol.
Symbol:	Data entry box to specify user-defined display symbol.

Displaying probe interaction results

Probe Interaction calculates empirical energy field maps, called brick maps, and displays them. A probe is used to sample the environment of the displayed structure. The probe is a point charge with van der Waals characteristics. As the structure is sampled, the energy is calculated between the probe and the structure at all points within a sampling box.

The energy calculated is the van der Waals energy, the electrostatic energy, or the sum of both energies. The van der Waals energy is calculated using the atom types currently assigned. The electrostatic energy is calculated using the charges currently assigned to the atoms.

The results of the calculation are written into a specified file, *filename.mbk*, and a brick map is displayed as a graphical object. The number of contours contained in this map and the color of each contour can be changed within QUANTA. The map can be displayed automatically on completion of the calculation, or at a later time.

In this section, empirical energy field maps are calculated for the interaction of a proton with nitrobenzene (nitrobenzene.msf). Procedures include:

- Setting up probe and molecule interaction calculations
- Displaying results as brick maps
- Manipulating graphical objects
- Adjusting contour colors and levels

Complete the following exercise to become familiar with the procedure for generating and manipulating a brick map.

1. Start a Probe Interaction calculation.

Display the **Calculate** menu and select **Interaction Maps**. From the pull-right menu that opens, select **Probe**. A dialog box offers probe interaction options. See [Table 31](#) for a list of the options and a brief description of each.

Select the options:

Wait for Calculation to Complete
van der Waals + Electrostatics

Enter the values:

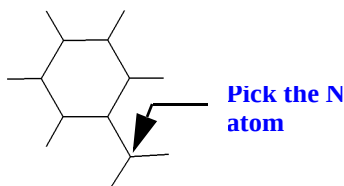
Probe Name: prot (four letters only)
Probe Charge: 1.0
Box Dimensions (angstroms): 10
Grid Size (angstroms): 0.5
Maximum Energy: 100
Minimum Energy: -100

Select the option:

Center on an Atom

Click the **OK** button and the message line reads:

Pick one atom - Pick any palette tool to quit.
 Pick atom for center of box.



Pick the nitrogen atom in the structure. A File Librarian dialog box requests a name for the brick map file (.mbk). In the text entry field, enter the text:

nitrobenzene

Click the **Save** button. The calculation starts and the cursor arrow changes to a wait watch.

2. Display the brick map as a graphical object.

6. Using Graphical Objects

When the calculation of the brick map is completed, a dialog box requests a name for the map graphical object. Enter the name:

probemap1

Click the **OK** button. A dialog box offers options for selecting the area of the brick map to be displayed.

Select the option:

All of the map displayed

Click the **OK** button. A dialog box asks for the number of contour levels to map.

Enter the value:

Enter the integer: 2

Click the **OK** button. A dialog box offers options for specifying the values and colors for each contour level.

Enter the level values:

1st contour level: -4.0

2nd contour level: 2.0

Enter the color numbers:

1st contour color: 14

2nd contour color: 13

Click the **OK** button and the brick map is displayed using the new contour values and color specifications. The energy value at grid intersections in each contour is displayed in the grid's associated color in the lower-right corner of the viewing area. You may wish to scale down the display using the Dial Emulator to see the entire surface.

The brick map object can also be created by selecting **Create Objects** from the **Draw** menu.

3. Delete the brick map object.

In the Object Management Table, toggle the **Delete** cell of the probemap1 object from **no** to **yes**. The surface is deleted from the viewing area, but the file nitrobenzene.mbk is not deleted. The brick map is deleted and no longer displayed.

Table 31. Probe interaction options

Option	Description
Wait for Calculation to Complete	Runs the probe interaction calculation as a foreground process. No modeling operations are performed until the surface is calculated.
Don't Wait; Run in Background	Runs the probe interaction calculation in the background. Other tasks can be performed during the calculation. Show Status in the Calculate menu enables you to determine when the job is done. Create Objects in the Draw menu displays the surface when the calculation is done.
Calculation	
van der Waals Calculation	Includes only the van der Waals term when calculating the energy.
Electrostatics Calculation	Includes only the electrostatics term when the energy is calculated.
van der Waals + Electrostatics	Includes both the van der Waals term and electrostatics terms when calculating the energy.
Use distance dependent dielectric	Modifies the dielectric “constant” to be a function of distance.
Probe Name	Specifies an atom type, typically water (WATE), methane (METH), oxygen (OXYG), or a proton (PROT) to be a probe. The probes are defined in the file \$HYD_LIB/param.par. Any valid CHARMM atom type in the file can be used as a probe.
Probe Charge	Specifies a charge for the probe. Any value can be entered to specify integer or partial charges.
Box Dimensions (Angstroms)	Specifies the length of each side of the square sampling box.
Grid Size (Angstroms)	Specifies the mesh size used when generating the brick map. The default value, 0.5 Å, is appropriate for small molecules. Larger molecules may require a larger mesh size (2.0 Å).
Maximum Energy	Sets the maximum energy value. Any calculated energies that are greater than the maximum energy are set to this value.
Minimum Energy	Sets the minimum energy value. Any calculated energies that are less than the minimum energy are set to this value.
Center on an Atom	Specifies an atom position as the center of the sampling box used in the calculation.
Center at a Coordinate	Specifies a coordinate location as the center of the sampling box used in the calculation

Displaying molecule interaction results

The Molecule Interaction function computes the interaction between two molecules: a probe and a target. The interaction energy between probe and target is the sum of two nonbond interactions:

6. Using Graphical Objects

- van der Waals (Lennard–Jones term).
- Electrostatic.

The probe molecule is tumbled about the target at specified angles and increments. An energy calculation is performed at each point of a grid superimposed on the target, using all possible combinations of probe rotation angles. A contour map is computed by taking the minimum energy value from each grid point. For fine grids or small rotation increments, the molecule interaction calculation can be lengthy. For example, for a probe tumble angle of 60°, 216 energy calculations are performed at each grid point.

The electrostatic and van der Waals interactions of a probe molecule, water, and target molecule, search1.msf, are calculated in the following exercise and displayed as brick maps. The structure, search1, was constructed in Chapter 2. If you did not complete the exercises in Chapter 2, do so before proceeding with this exercise.

1. Build a water molecule probe.

Display the **Applications** menu, select **Builders**, and then select **2D Sketcher** from the pull-right menu. In the ChemNote window that opens, place an O (oxygen) atom in the viewing area. The **2D** function automatically adds the appropriate hydrogens.

Display the ChemNote **File** menu and select the **Return to Molecular Modeling** function. A dialog box asks if the changes should be saved.

Click the **Yes** button. In the File Librarian dialog box that opens, enter the text:

water

Click the **Save** button. The ChemNote window is removed from the screen and a dialog box offers options for displaying MSFs.

Select the option:

Use the new molecule water.msf only

Click the **OK** button and the structure stored in water.msf is displayed.

2. Open the target molecule file (search1.msf).

Display the **File** menu and select **Open**. In the Open MSF File Librarian dialog box, select the file search1.msf from the scrolling list.

Select the option:

Append

Click the **Open** button and both the water molecule and the search1 molecule are displayed in the viewing area.

Select **Reset View** from the Geometry palette to reposition the MSFs in the center of the viewing area.

3. Set up the molecule interaction calculation.

Display the **Calculate** menu and select **Interaction Maps**. From the pull-right menu that opens, select **Molecule** and the Molecular Interaction Grid dialog box opens. See [Table 32](#) for a list of the options and a brief description of each.

Select the options:

Wait for Calculation to Complete
van der Waals + Electrostatic

Enter the values:

Probe Tumble Increment: 180
Box Dimensions (Angstroms): 15
Grid Size (Angstroms): 1
Maximum Energy: 100
Minimum Energy: -100

Select the option:

Center on an atom

Click the **OK** button. The 180° increment and 1 Å grid size expedite the calculation. Values in the vicinity of 60° and 0.1 Å are more typically used in accurate molecule interaction calculations.

4. Define the atom to be the center of the box.

A message in the message line reads:

Pick an atom - Pick any palette tool to quit. Pick an atom for center of box.

Pick the search1.msf ring carbon that is the connection point for the longest branch. In the File Librarian dialog box that opens, enter the name of the brick map.

Enter the text:

mol_inter

Click the **Save** button.

5. Select the probe molecule and begin calculation.

6. Using Graphical Objects

In the dialog box that asks for which molecule to display, select the structure:

water.msf

Click the **OK** button. The calculation begins and the cursor changes to a watch until the calculation finishes in approximately 10 minutes, depending on the hardware. When the calculation is complete, a dialog box is asked you to choose a save option.

Select:

Create New Generation of water.msf

The structure is saved and the textport reads:

```
The old structure is renamed water.msf,001
```

6. Display the brick map.

A dialog box asks for the name of the map just calculated. Enter the name:

probemap2

Click the **OK** button. A dialog box asks which molecule to attach the interaction map to.

Select search1.msf from the scrolling list.

Click the **OK** button. A dialog box offers options for selecting the area of the brick map to be displayed.

Select the option:

All of the map displayed

Click the **OK** button. A dialog box asks for the number of contour levels to map.

Enter the value:

Enter the integer: 2

Click the **OK** button. A dialog box offers options for specifying the values and colors for each contour level.

Enter the level values:

1st contour level: -3

2nd contour level: 3

Enter the color numbers:

1st contour color: 7

2nd contour color: 8

Click the **OK** button.

Calculation time depends on the hardware, but is usually short. When the calculation is complete, a brick map of the contours is displayed. The low-energy attractive regions of the surface are displayed in color 7, default green. High-energy repulsive regions are displayed in color 8, default purple.

Rotate and translate the structure to observe the relationships between chemical structure and contour shape.

7. Delete the brick map object.

In the Object Management Table, toggle the **Delete** cell of the mol_inter object listing from **no** to **yes**. The surface is deleted from the viewing area, but the file mol_inter.mbk is not deleted.

8. Reconstruct a brick map.

Brick maps and other graphic objects are not saved when QUANTA is exited. However, graphic objects, a brick map in this case, can be reconstructed without repeating the calculation.

Display the **Draw** menu and select **Create Objects**. In the Graphic Object Generation Options dialog box that opens, select the option:

Brick Maps

Enter the values:

Object Name: probemap1

Object Color (1-14): 1

Select the option:

Attack to MSF

Select search1.msf from the scrolling list.

Click the **OK** button. From the scrolling list in the File Librarian dialog box, select mol_inter.mbk, and then click the **Open** button.

In the new dialog box that is opens, select the option:

All of the map displayed

Click the **OK** button. In the contour level dialog box that opens, enter the value:

2

6. Using Graphical Objects

Click the **OK** button. In a dialog box for entering the contour levels and color numbers, note the minimum and maximum values reported, and enter the values:

1st Contour: -3

2nd Contour: 3

1st Contour Color: 7

2nd Contour Color: 8

Click the **OK** button and a brick map of the contours is displayed. The low-energy attractive regions of the surface are displayed in color 7, default green. High-energy repulsive regions are displayed in color 8, default purple.

Rotate and translate the structure to observe the relationships between chemical structure and contour shape.

9. Delete the brick map object.

In the Object Management Table, toggle the **Delete** cell of the mol_inter object listing from **no** to **yes**. The surface is deleted from the viewing area, but the file mol_inter.mbk is not deleted.

Calculating electrostatic interactions only

You can calculate and generate a brick map display based on electrostatic interactions, ignoring van der Waals interactions.

Complete the following exercise to show the interaction of a water molecule with search1.msf, without van der Waals interactions being modeled in the calculation.

1. Start the molecule interaction calculation.

Display the **Calculate** menu and select **Interaction Maps**. Then select **Molecule** from the pull-right menu that opens and the Molecular Interaction Grid dialog box opens. See [Table 32](#) for a list of the options and a brief description of each.

Select the options:

Wait for Calculation to Complete
Electrostatic Calculation

Enter the values:

Probe Tumble Increment: 180

Box Dimensions (Angstroms): 10

Grid Size (Angstroms): 1

Maximum Energy: 100

Minimum Energy: -100

Select the option:

Center on an atom:

Click the **OK** button and the 180° increment 1 Å grid size expedite the calculation. Values in the vicinity of 60° and 0.1 Å are more typically used in accurate molecule interaction calculations.

A message in the message line reads:

Pick any atom - Pick any palette tool to quit.
Pick an atom for center of box.

Using the mouse, select the same ring carbon used in the previous calculation.

A File Librarian dialog box asks for the name for the map file. Enter the filename:

electro1.mbk

Click the **Save** button and a dialog box asks which molecule is the probe. From the scrolling list, select:

water.msf

Click the **OK** button. The calculation begins and the cursor changes to a watch. When the calculation is complete, a dialog box asks you to choose a save option.

Select:

Create New Generation of water.msf

The structure is saved and the textport reads:

The old structure is renamed water.msf,002

2. Display the brick map as a graphical object.

When the calculation of the brick map is completed, a dialog box requests a name for the map graphical object.

Enter the name:

electro1

Click the **OK** button and a dialog box opens for attaching the graphical object to an MSF. Select the scrolling-list entry:

search1

6. Using Graphical Objects

Click the **OK** button. A dialog box offers options for selecting which area of the brick map to display.

Select the option:

All of the map displayed

Click the **OK** button and a dialog box asks for the number of contour levels to map.

Enter the value:

Enter the integer: 1

Click the **OK** button and a dialog box offers options for specifying the values and colors for each contour level.

Enter the level values:

1st contour level: -50

Enter the color numbers:

1st contour color: 12

Click the **OK** button. The brick map is displayed with electrostatic interactions in contours of light blue.

3. Delete the brick map object.

In the Object Management Table, toggle the **Delete** cell of the electro1 object listing from **no** to **yes**. The surface is deleted from the viewing area, but the file electro1.mbk is not deleted.

Table 32. Molecular probe interaction options

Option	Description
Wait for Calculation to Complete	Runs the probe interaction calculation in the foreground. No other operations are performed until the surface is calculated.
Don't Wait; Run in Background	Runs the probe interaction calculation in the background. Modeling tasks can be performed while the surface is being calculated. Show Status in the Calculate menu makes it possible to determine when the job is done. Create Objects in the Draw menu displays the surface when the calculation is completed.

Calculation

van der Waals Calculation Includes only the van der Waals term when calculating the energy.

Electrostatics Calculation Includes only the electrostatics term when the energy is calculated.

van der Waals + Electrostatics Includes both the van der Waals term and electrostatics terms when calculating the energy.

Table 32. Molecular probe interaction options (Continued)

Option	Description
Use Distance Dependent Dielectric	Modifies and uses the dielectric “constant” as a function of distance.
Probe Tumble Increment	Specifies the tumble increment parameters for the probe.
Box Dimensions (Angstroms)	Specifies the length of each side of the square sampling box.
Grid Size (Angstroms)	Specifies the mesh size used when generating the brick map. The default value, 0.5 Å, is appropriate for small molecules. Larger molecules may require a larger mesh size (2.0 Å).
Maximum Energy	Sets the maximum energy value. Any calculated energies that are greater than the maximum energy are set to this value.
Minimum Energy	Sets the minimum energy value. Any calculated energies that are less than the minimum energy are set to this value.
Center on an Atom	Specifies an atom position as the center of the sampling box used in the calculation. A dialog box is displayed, enabling the selection of the atom.
Center at a Coordinate	Specifies a coordinate location as the center of the sampling box used in the calculation. A dialog box opens for specifying the coordinate location.

Managing maps

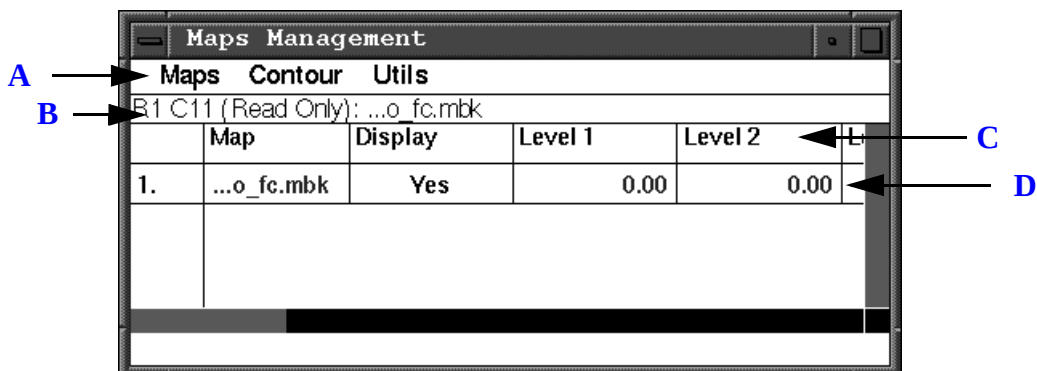
The Maps Management table provides an interface to the general-purpose volume visualization capabilities of QUANTA. 3D volume information is stored in brick maps, which are used for storing electron density, molecular probe maps, volumes, electrostatic potential, and molecular surface information generated within QUANTA. In addition, the maps can be generated by external programs for display within QUANTA. The molecular or volume properties that these maps contain are displayed within QUANTA as chicken-wire contours or solid surfaces.

The Maps Management table is available in any application in QUANTA and provides a spreadsheet-like interface to tools that manage and display the 3D information held in QUANTA brick map files. Its display can be turned on or off using the **Map Table** pull-right menu on the **Draw** menu. These tools convert map formats to QUANTA-compatible brick maps and define active maps, contour levels and display styles. Additional tools save and retrieve the contents of brick map display lists and purge the brick map database of undisplayed bricks to reduce memory requirements.

The following figure shows the Maps Management table. The table has the following components:

6. Using Graphical Objects

- Its own menu bar of commands (A on the figure).
- An edit line in which the contents of the currently selected cell is displayed (B on the figure).
- A column heading line (C on the figure).



Some tools available on the Maps Management table are *not* relevant within X-LIGAND, X-SOLVATE, X-AUTOFIT, X-POWERFIT, and X-BUILD. These applications automatically control the map display; changes to some general map options can interfere with the tools' use of the maps, with serious detriment to speed and results. Please refer to the *X-Ray Structure Analysis User's Guide* for further details if you use these applications.

Generating an electrostatic potential energy surface

The **Electrostatics** selection in the **Calculate** menu provides the ability to calculate and display an electrostatic potential energy surface on a molecule in either:

- 3D surface mode.
- 2D isoenergetic contour plot mode.

The electrostatic potential can be calculated using partial atomic charges obtained from a previous CHARMM calculation or with the VSS method based on the work of Giessner-Prettre and Pullman. (See Method II described in citation 6 in the References section of this chapter.) 3D potentials can be displayed as a grid map or a dot matrix.

On the electrostatic potential grid map, large negative potential contours correspond to very electronegative regions on the van der Waals surface and appear where negative partial atomic charges control the electrostatic potential. Regions corresponding to positive electrostatic potential occur where the resulting charge is positive. A color-coded scale of electrostatic potential is listed in the lower-right corner of the viewing area. The color display scale can be adjusted to fit the data for the displayed structure.

A dot matrix display uses dots to outline the van der Waals surface. Color may also be used to display areas of relative electronegativity or positivity.

Calculating and displaying an electrostatic potential grid map

Complete the following exercise to build the structure cyclohexanol and then generate an electrostatic grid map for it:

1. Create cyclohexanol using ChemNote.

Display the **Applications** menu, select **Builders**, and then select **2D Sketcher** from the pull-right menu that opens. In the ChemNote window, sketch the structure cyclohexanol, using appropriate bond, ring, and atom selections. If you have never used ChemNote, complete the exercises in Chapter 1 to become familiar with its operations.

2. Return the cyclohexanol structure to Molecular Modeling.

Display the ChemNote **File** menu and select **Return to Molecular Modeling**. A dialog box asks if the changes should be saved.

Click the **Yes** button. In the File Librarian dialog box that opens, enter the text:

cyclohexanol

Click the **Save** button. The ChemNote window is removed from the screen, and a dialog box offers options for displayed MSFs.

Select the option:

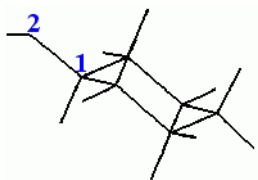
Use the new molecule cyclohexanol.msf only

Click the **OK** button and the structure is displayed in the viewing area.

Rotate the structure to visualize the orientation of the hydroxyl hydrogen relative to the ring atoms.

3. Move the hydroxyl hydrogen.

6. Using Graphical Objects



From the **Modeling** palette, select **Torsions**. The **Select Torsions** palette is displayed and the message line reads:

Pick 1st atom defining torsions or pick FINISH to continue

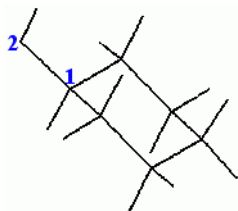
Pick the carbon atom attached to the oxygen and the message line reads:

Pick 2nd atom defining torsions or pick FINISH to continue

Pick the oxygen atom as the second atom involved in the torsional rotation and the message line reads:

Pick 3rd atom defining torsions or pick FINISH to continue

From the Select Torsions palette, select **Finish**.



Dial Set 3 is displayed in the Dial Emulator. Use the Torsion 1 dial to rotate the hydroxyl hydrogen to a position in which it is *trans* (180°) to the hydrogen on the carbon that is attached to the hydroxyl oxygen. Ignore the numbers in the lower left of the viewing area.

4. Save the torsion changes.

From the Modeling palette, select **Save Changes**. A dialog box offers options to save the new coordinates of cyclohexanol.msf.

Select the option:

Overwrite cyclohexanol.msf

Click the **OK** button and the coordinates are saved.

5. Minimize the structure.

Display the **CHARMm** menu and select **Minimization Options**. A dialog box offers minimization setup options.

Select the option:

Newton Raphson

Enter the values:

Number of Minimization Steps: 15

Coordinate Update Frequency: 1

Energy Gradient Tolerance: 0.000001

Energy Value Tolerance: 0

Initial Setup Size: 0.02

Step Value Tolerance: 0

Click the **OK** button and the new minimization parameters are established.

From the Modeling palette, select **CHARMm Minimization**. The CHARMm calculation is begun and stops when the rms force is less than 0.000001.

6. Save the minimization changes.

From the Modeling palette and select **Save Changes**. A dialog box offers the option to save the new coordinates of cyclohexanol.msf.

Select the option:

Overwrite cyclohexanol.msf

Click the **OK** button and the minimized coordinates are saved.

7. Calculate electrostatic potential.

Display the **Calculate** menu and select **Electrostatic**. From the pull-right menu, select **Potential** and the Calculate Electrostatic Potential palette is displayed.

Select **Calculate 3D Surface**, **Calculate from Partial Charges**, and **3D Surface Parameters**.

From the Setup 3-D Surface Parameters dialog box, select the default options:

Reentrant

Solvent Probe Radius: 1.4

Medium

Big Dots

Grid Contour Mesh

Click the **OK** button.

8. Run electrostatic potential.

From the Calculate Electrostatic Potential palette, select **Run and Wait**. In the File Librarian dialog box that opens, enter the text:

3dcyclo

Click the **Save** button. The electrostatics calculation starts and the cursor changes to a watch. You can follow the calculation status in the textport. When the calculation is completed, the cursor returns to an arrow.

9. Display the results.

From the Calculate Electrostatic Potential palette, select **Display Results**. The Display Potentials palette and a File Librarian dialog box are displayed.

From the File Librarian, select the 3dcyclo.epo file and then click the **Open** button.

From the Display Potentials palette, select **Show 1-Molecule Potential** and a dialog box opens for entering an object label.

Enter the name:

potential1

and click the **OK** button. A grid map appears in colors described in the color scale in the lower-right corner of the viewing area. The colors indicate the potential near the surface of the molecule.

The Object Management Table opens listing the object, potential1, and its status.

10. Reset the contour scale.

In the Display Potentials palette, select **Set Contour Levels** and a dialog box opens with a set of eight **Potential Value** data entry fields. The minimum and maximum potential values (in units of kcal/mol) for the simulation are reported at the top of the dialog box. These values can be used to create more realistic contour values.

Referring to the values at the top of the box, enter the value for the **Minimum Value of Potential** in the **Potential Value 1** data entry field.

Enter the value for the **Maximum Value of Potential** in the **Potential Value 8** data entry field. These are the upper and lower limits for the potentials of the electrostatic field for cyclohexanol in this calculation.

Click the **Auto Scale** button. The values in the **Potential Value 2** through **Potential Value 7** boxes are automatically incremented

between the minimum and maximum potential values that you enter. You can also set values 2 through 7 manually.

Click the **OK** button to display the contours using the new values.

From the Display Potentials palette, select **Finish**. The Display Potentials palette is closed and the Calculate Electrostatic Potentials palette is redisplayed.

Calculating and displaying an electrostatic potential dot surface

The electrostatic potential can also be displayed as a dot surface. The dot surface electrostatic potential is calculated and displayed in the same manner as the electrostatic potential grid map.

Complete the following exercise to display a dot surface electrostatic potential for cyclohexanol.

1. Set up a dot surface electrostatic potential.

Display the Calculate Electrostatic Potentials palette.

Select **Calculate 3D Surface**, **Calculate from Partial Charges**, and **3D Surface Parameters**.

In the Setup 3-D Surface Parameters dialog box that opens, select the option:

Reentrant

Enter the value:

Solvent Probe Radius: 1.4

To specify density points, select the option:

Medium

To specify surface representation, select the option:

Dot Surface

To specify the type of dot symbol, select the option:

Big dots

Click the **OK** button.

2. Run the electrostatic potential.

6. Using Graphical Objects

From the Calculate Electrostatic Potential palette, select **Run and Wait**. In the File Librarian dialog box that opens, enter the text:

points

Click the **Save** button. The electrostatics calculation starts and the cursor changes to a watch. You can view the calculation status in the text-port. When the calculation is completed, the cursor returns to an arrow.

3. Display Results.

From the Calculate Electrostatic Potential palette, select **Display Results**. The Display Potentials palette and a File Librarian dialog box are displayed.

Select the points.epo file from the File Librarian and then click the **Open** button.

From the Display Potentials palette, select **Show 1-Molecule Potential**. In the dialog box that opens for entering an object label, enter the name:

potential2

and click the **OK** button. A dot surface appears in several colors over the cyclohexanol structure. A color-coded potential values scale (in kcal/mol) is displayed in the lower-right corner of the viewing area.

4. Reset the contour scale.

In the Display Potentials palette, select **Set Contour Levels**. A dialog box offers a set of eight **Potential Value** data entry fields. The minimum and maximum potential values (in units of kcal/mol) for the simulation are reported at the top of the dialog box. These values can be used to create more realistic contour values.

For example:

Enter the value for the **Minimum Value of Potential** in the **Potential Value 1** data entry field. Enter the value for the **Maximum Value of Potential** in the **Potential Value 8** data entry field. Click the **Auto Scale** button:

Click the **OK** button to display the contours using the new values.

5. Hide the point map.

From the Display Potentials palette select **Finish**. The Display Potentials palette is replaced by the Calculate Electrostatic Potential palette.

Select the **Displayed** column for potential2 in the Object Management Table. The dot surface is removed from the viewing area. Objects potential1 and potential2 are both hidden but still attached to the cyclohexanol structure.

Calculating and displaying an isoenergy 2D contour plots

A 2D isoenergetic contour plot can be calculated and displayed using a method similar to that for generating grid maps and dot surfaces.

Complete the following exercise to calculate and display this type of object.

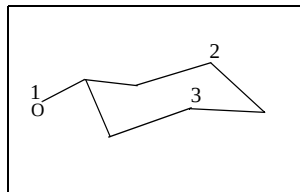
1. Set up a 2D contour plot for cyclohexanol.

From the Calculate Electrostatic Potential palette, select **Calculate 2-D slice**, **Calculate from Partial Charges**, and **Define Plane**.

The message line prompts you to pick three atoms in the molecule to define the plane of interest:

Pick one atom — other input disabled. Pick three atoms to define plane.

From the Select palette, select the cyclohexanol atoms 1, 2, and 3, as indicated in the figure below. When the third atom is selected, the structure is reoriented so the selected plane is parallel to the screen. The Select palette is removed from the screen.



2. Define the zero plane.

From the Calculate Electrostatic Potential palette, select **Run and Wait**. A box requests that you specify the atom upon which the zero plane will be defined.

Click the **Interactive** button and the message line reads:

Pick one atom — pick any palette tool to quit.
Pick atom instead of typing.

Pick one atom to define the center of the plane. When you make your pick, a File Librarian dialog box requests the name for a new output file.

6. Using Graphical Objects

Enter the text:

2dpartial

Click the **OK** button and the calculation proceeds. The cursor appears as an arrow to a watch until the calculation is complete.

3. Display the results.

Select **Display Results** from the Calculate Electrostatic Potential palette and a File Librarian dialog box opens.

Select the file 2dpartial.epo and click the **Open** button. A dialog box asks you to save or reject the current model. Select **Save**.

From the Calculate Electrostatic Potential palette, select **Show 1-Molecule Potential**. In the File Librarian dialog box that opens, enter the name potential3 and click the **OK** button. A 2D contour plot appears in several colors. A color-coded potential values scale (in units of kcal/mol) is displayed in the lower-right corner of the viewing area.

4. Reset the contour scale.

In the Display Potentials palette, select **Set Contour Levels**. A dialog box offers a set of eight Potential Value data entry fields. The minimum and maximum potential values (in units of kcal/mol) for the simulation are reported at the top of the dialog box. These values can be used to create more realistic contour values.

In the **Potential Value 1** data entry field, enter the value for the **Minimum Value of Potential**. In the **Potential Value 8** data entry field, enter the value for the **Maximum Value of Potential**. Click the **Auto Scale** button.

Click the **OK** button to display the contours using the new values.

5. Hide the 2D contour plot object.

From the Display Potentials palette select **Finish**. The Display Potentials palette is replaced by the Calculate Electrostatic Potential palette.

Select the **Display** column for 2dpartial in the Object Management Table. The text changes from **no** to **yes** and the 2D contour plot is removed from the viewing area. No objects are displayed with cyclohexanol.

Generating an electrostatic field

Electrostatic field calculations are performed using the fieldcalc program developed by F. Blaney. The electrostatic field is calculated using essentially the same procedure as employed for the electrostatic potential. The calculated field is shown as colored arrows.

Complete the following exercise to become familiar with the procedure for calculating and displaying an electrostatic field.

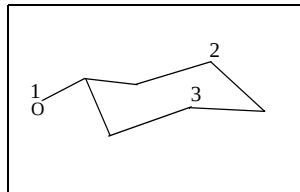
1. Set up an electrostatic field calculation.

Display the **Calculate** menu and select **Electrostatic**. From the pull-right menu that opens, select **Field**.

From the Calculate Electrostatic Field palette, select **Calculate 2-D Slice**, **Calculate from Partial Charges**, and **Define Plane**.

The message line prompts you to select the three atoms that define the plane on which the electrostatic field is displayed:

Pick one atom — other input disabled. Pick three atoms to define plane.



From the **Select** palette that is displayed, select the cyclohexanol atoms 1, 2, and 3, as indicated in the figure above. When the third atom is selected, the structure is reoriented so the selected plane is parallel to the screen. The Select palette is removed from the screen.

2. Define the zero plane.

From the Calculate Electrostatic Field palette, select **Run and Wait**. A dialog box requests that you specify the atom upon which the zero plane will be defined.

Click the **Interactive** button and the message line reads:

Pick one atom — pick any palette tool to quit.
Pick atom instead of typing.

6. Using Graphical Objects

Pick one atom to define the center of the plane, and a File Librarian dialog box requests the name for a new output file.

Enter the text:

2dfield

Click the **Save** button.

3. Display the results.

When the calculation is complete, select **Display Results** from the Calculate Electrostatic Field palette. In the File Librarian dialog box that opens, select the file 2dfield.efo and click the **Open** button. A dialog box asks you to save or reject the current model.

Select **Save** and the Display Field palette allows you to modify vector arrow size and exclude small vectors to simplify the plot.

Select **Display Field**. In the File Librarian dialog box that opens, enter the name field1 and click the **OK** button. A vector field of arrows of different size, color, and direction are displayed. Larger arrows indicate greater field magnitudes, with a blue arrow indicating a negative field and a red arrow indicating a positive field.

From the Display Field palette, select **Finish**. From the Calculate Electrostatic Field palette, select **Finish**. The Modeling palette is displayed.

4. Delete all objects.

Select the title cell for the **Delete** column in the Object Management Table. The vector field is removed from the viewing area and all objects are deleted from the Object Management Table. The table closes.

Generating and displaying hydrogen bonds

Although hydrogen bonds are generated and displayed like the graphical objects discussed in other sections of this chapter, hydrogen bonds are handled quite differently.

The hydrogen bond function searches a displayed structure for possible hydrogen bonds and monitors the interaction of a molecular structure with a substrate. In the QUANTA **Calculate** menu, **Hydrogen Bond** calculates and displays hydrogen bonds any time the structure is changed. The presence or absence of a hydrogen bond is evaluated by whether the prospective atoms meet defined distance and angle criteria.

In the Modeling palette, **Hydrogen Bond** performs a one-time calculation of hydrogen bonds for the displayed structure and displays the results. Hydrogen bonds are indicated by dashed white lines between the involved atoms.

The hydrogen bond function relies on information in the atom parameter file that indicates whether a particular type of atom is a potential hydrogen bond donor or acceptor. The parameter file contains a hydrogen bond column for each atom type, consisting of one of four letters that indicate the hydrogen-bonding capability of a particular atom type. The letters are:

- D for donor
- A for acceptor
- E for either donor or acceptor
- N for neither donor or acceptor

A polar hydrogen atom is flagged as a donor. When hydrogen atoms are not included in atom data files, atoms attached to polar hydrogen atoms are flagged as donors.

In checking hydrogen bond geometry, the hydrogen bond function considers the donor and acceptor atoms as well as the atoms bonded to the donor and acceptor. Criteria used in checking geometry are:

- The separation of the two hydrogen bonding atoms must be less than a specified limit.
- The angles between groups of three atoms must be greater than a specified limit.

The limit values can be listed and changed using **Bond Options** in the **Edit** menu. Parameters are designated as: d1don, d2don, d1hyd, d2hyd, ang1d, angla, and anglh.

The default values for these parameters are shown in [Table 33](#).

Table 33. Default values for hydrogen bond parameters

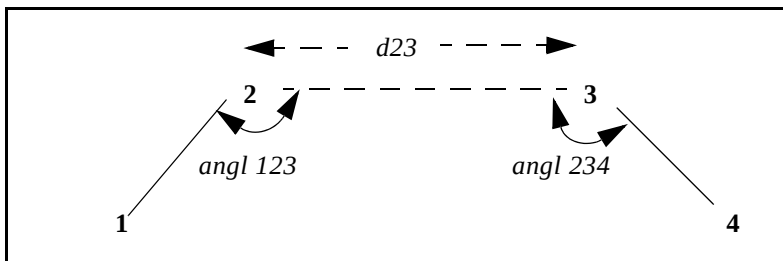
Distance	Angle
d1hyd = 2.5	angla = 90°
d2hyd = 3.0	anglh = 90°
d1don = 3.3	angld = 90°
d2don = 4.0	angld = 90°

6. Using Graphical Objects

The distance criteria for d2don and d2hyd are greater than for d1don and d1hyd. These criteria are used as the limit for near- hydrogen bonds to be listed to a file. Near-hydrogen bonds are potential hydrogen bonds that do not satisfy the strict criteria to be hydrogen bonds, but have appropriate chemical groups sufficiently close to the distance and angle limits to be considered possible hydrogen bonds. The d2don parameter is used in the same situation as d1don.

The default parameters used in QUANTA are based on the results of the analysis of hydrogen bonding in proteins. See citation 5 in the Reference section at the end of this chapter.

All hydrogen bonds, including near-hydrogen bonds and changes in defaults, can be displayed on screen and listed to a file. In the file, QUANTA lists the atoms used in calculating the hydrogen bond geometry, the angles (see *angl 123* and *angl 234* in the figure below), and distances (see *d23* below). If all atom are not defined, some angles and distances are not calculated.

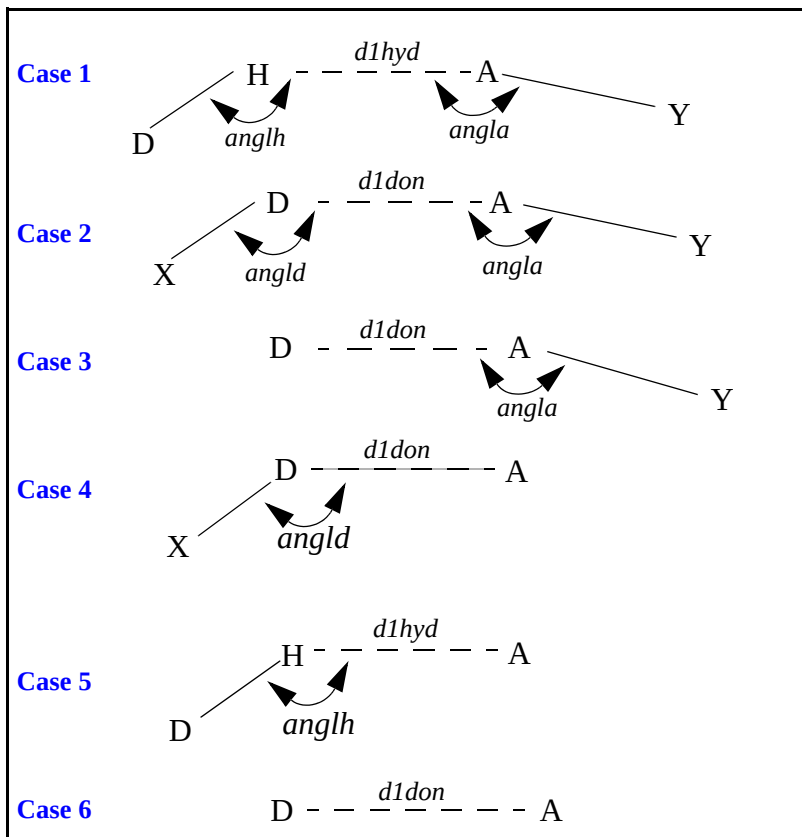


Various situations are possible for hydrogen bonding. For example, the atoms attached to a donor or acceptor may not be defined. The next figure illustrates several situations where hydrogen bonding may occur.

In this figure, atoms are labeled:

- H for hydrogen atoms
- D for non-hydrogen atom donors
- A for acceptors
- X for atoms bonded to donor
- Y for atoms bonded to acceptor

The interatomic distances and angles that are calculated in the geometry checking are indicated and labeled with the name of the limiting value.



In Cases 1 and 2, four atoms define the geometry. In Case 1, the hydrogen atom is defined. In Case 2, it is not. In both these cases, a distance criterion and two angle criteria are applied.

In Cases 3 through 5, three atoms define the hydrogen bond geometry. Therefore, only one bond angle criterion can be applied.

In Case 6, only two atoms are defined. Therefore, only the distance criterion can be applied.

Complete the following exercise to become familiar with procedures to calculate, display, and save hydrogen bonds. Bond angle and distance criteria are changed, which changes the number of hydrogen bonds calculated.

Use *mypeptide.msf* for this exercise. The structure was constructed in the section, *Creating a Peptide*, in Chapter 4. If you did not complete this section, do so before proceeding.

6. Using Graphical Objects

1. Open mypeptide.msf.

Display the **File** menu and select **Open**. In the Open MSF File Librarian dialog box that opens, select mypeptide.msf from the scrolling list.

Select the option:

Replace

Click the **Open** button to display the structure in the viewing area.

2. Start the Hydrogen Bonds application.

Display the **Calculate** menu and select **Hydrogen Bonds**. The Hydrogen Bonds palette is displayed. See Table 33 for a list of the selections in this palette and a brief description of each.

3. Set the hydrogen bond parameters.

From the Hydrogen Bonds palette, select **Set Parameters**. In the Set up hbond parameters dialog box that opens, enter the values:

Max distance between hydrogen atom and acceptor: 2.5

As above but for “near” hydrogen bonds: 3.0

Max distance between atom bearing hydrogen and acceptor: 3.3

As above but for “near” hydrogen bonds: 4.0

Minimum angle at the acceptor: 90.0

Minimum angle at the hydrogen: 90.0

Minimum angle at the atom bearing the hydrogen: 90.0

Click the **OK** button.

4. Calculate and display hydrogen bonds.

From the Hydrogen Bonds palette, select **Calculate Hbonds**. Dashed white lines connect atoms that are calculated to meet the default distance and geometry criteria set up in the hbond parameters dialog box. **Show Hbonds** is automatically selected.

5. Hide hydrogen bonds.

From the Hydrogen Bonds palette, select **Show Hbonds** to turn it off. The dashed lines disappear and the selection is no longer highlighted.

6. Write the list of hydrogen bonds to a file.

From the Hydrogen Bonds palette, select **List to File**. A File Librarian dialog box prompts you for a filename. Enter the name: mypeptide.

Click the **Save** button and a dialog box asks for a title for the hbond file. Click the **OK** button to indicate there is no title for this file. The hydrogen bond information is stored in mypeptide.hbo.

The list of hydrogen bonds is written out to an ASCII file:

DONOR				ACCEPTOR													
SEG	RES	ATOM1		ATOM2	ATOM3	ATOM4		RES	SEG	A123	D23	A234	ACON	DON	AHNO		
ATPP	ILE	16	N	16	HT2	143	O	143	C	ASN	ATPP	132.9	2.06	140.2	128.6	2.87	31.7
ATPP	ILE	16	N	16	HT3	194	OD1	194	CG	ASP	ATPP	127.6	1.85	106.3	123.4	2.61	34.1
ATPP	VAL	17	N	17	H	189	O	189	C	ASP	ATPP	149.0	1.96	164.9	170.7	2.88	20.5
&ATPP	VAL	26	C	27	N	717	O			HOH	ESOL	140.0	2.84			0.00	S S
&ATPP	TYR	29	CZ	29	OH	499	O			HOH	ESOL	115.2	2.85			0.00	S S

Each line of this file reports a different hydrogen bond. The atoms defining the donor are listed first, followed by the acceptor atom(s).

The columns are labelled as:

An & symbol in column 3 signifies that the hydrogen bond is in the “near” list.

SEG - the segment name of the donor atom.

RES - the residue name of the donor atom.

ATOM1 - the name of the connecting atom in the donor group (Atom 1).

ATOM2 - the name of the donor atom in the donor group (Atom 2.)

ATOM3 - the name of the acceptor atom in the acceptor group (Atom 3).

ATOM4 - the name of the connecting atom in the acceptor group (Atom 4). (Atom 4 is not present for hydrogen bonds to waters). (Atom 1 is not present for hydrogen bonds from waters).

RES - the residue name of the acceptor atom.

SEG - the segment name of the acceptor atom,

A123 - the angle made between Atom1-Atom2-Atom3,

D23 - the distance between Atom2-Atom3,

A234 - the angle made between Atom2-Atom3-Atom4,

ACON - the angle made between Carbon, Nitrogen and Oxygen when they are in the Hbond (this is an additional measure emulating no-hydrogens on the protein).

DON - the distance between the oxygen and nitrogen (equivalent to ACON).

AHNO - the angle between the hydrogen, nitrogen and oxygen in a hydrogen bond.

The remaining symbols indicate whether the donor/acceptor are symmetry generated (S) or not ().

6. Using Graphical Objects

7. Display the hydrogen bond list on screen.

From the Hydrogen Bond palette, select **List to Screen**. The hydrogen bonds that meet the default criteria are reported in the textport.

8. Change the hydrogen bond parameters and recalculate.

From the Hydrogen Bonds palette, select **Set Parameters**. In the Set up hbond parameters dialog box, enter the values:

Max Distance between hydrogen atom and acceptor: 2.1

Minimum angle at the acceptor (Min 0 Max 180): 105

Leave all other parameters at their default values.

Click the **OK** button.

From the Hydrogen Bonds palette, select **Calculate Hbond** and the hydrogen bonds are recalculated.

9. Display the new hydrogen bond list on the screen.

From the Hydrogen Bonds palette, select **List to Screen**. Fewer hydrogen bonds are calculated as a result of tightening the distance and geometry criteria.

10. Exit Hydrogen Bonds.

From the Hydrogen Bonds palette, select **Finish** and a dialog box asks how the hydrogen bonds should be used.

Select the option:

No further hydrogen bond calculation

Click the **OK** button. The Hydrogen Bonds palette is removed from the screen, and the Modeling palette is redisplayed. **Hydrogen Bonds** is automatically selected in the Modeling palette, and the hydrogen bonds continue to be displayed.

From the Modeling palette, select **Hydrogen Bond**. The selection is turned off and the hydrogen bonds are deleted.

Applying settings to other structures

When you have established parameters, they can be applied to any structure by selecting **Hydrogen Bonds** in the Modeling palette.

Complete the following exercise to apply the hydrogen bond parameters to a different structure. The MSF newpeptide.msf was created by modifying the structure in the *Selecting Active Atoms* section of Chapter 2 in *QUANTA Basic Operations*. If you did not complete this exercise, do so before proceeding.

1. Open the new structure, newpeptide.msf.

Display the **File** menu and select **Open**. In the File Librarian dialog box that opens, select newpeptide.msf from the scrolling list. Select **Replace** and then select **Open** to display the structure in the viewing area.

2. Calculate the hydrogen bonds.

From the Modeling palette, select **Hydrogen Bonds** and the hydrogen bonds are calculated using the last specified parameters. The hydrogen bonds are displayed. See Table 34 for a list of the options and a brief description of each.

Select **Hydrogen Bonds** again to turn it off. The hydrogen bonds are deleted and **Hydrogen Bonds** is no longer highlighted.

Table 34. Hydrogen Bond palette

Selection	Description
Show Hbonds	Toggles the display of the hydrogen bonds (default is on). Has the same effect as the Hydrogen Bonds option in the Manage Display dialog box.
Calculate Hbonds	Calculates hydrogen bonds using the parameters and selection sets currently defined. If Show Bonds is selected, the bonds are displayed.
Edit Selection	Allows you to search for hydrogen bonds in a limited portion of the selected structure. Two sets of atoms can be defined. (The second set can be same as the first.) The sets are used in displaying and listing hydrogen bonds and remain in effect for the current QUANTA session only.
Include "Near" Hb	Toggles the inclusion of the near-hydrogen bonds in the list of hydrogen bonds.

Table 34. Hydrogen Bond palette (Continued)

Selection	Description
Inter/Intra Hbonds	Opens a dialog box offering options to exclude either intermolecular, intramolecular, intersegment, or intrasegment bonds.
Set Parameters	Sets the parameters to define hydrogen bonds. Parameters are used to display and list hydrogen bonds and are retained for future sessions until edited.
List to File	Bonds are listed to file (prompts for filename).
List to Screen	Bonds listed to textport.
Finish	Provides three options for finishing: 1. No further hydrogen bond calculation. 2. No further calculation, delete displayed hydrogen bonds. 3. Update hydrogen bonds when structure is updated. If option 3 is selected, the displayed hydrogen bonds are updated when Torsions or Move Fragment is active in the Modeling palette

Summary

Graphical objects are displayed in relation to but separate from the structures on which they are based. Although each object is a representation of data related to a structure, it is not part of the MSF. However, using the Object Management Table, you may attach an object to an MSF so that it can be moved and deleted with the structure. The Object Management Table also provides object display, naming, and deletion options. Each graphical object is uniquely identified so that you can manage it throughout a QUANTA session.

Some objects, such as ribbons and grid contour meshes, are generated within QUANTA. Other objects, such as brick maps, Connolly solvent surfaces, and 3D vectors, are generated from results of calculations outside of QUANTA.

Although hydrogen bonds are optionally generated and displayed the same as the graphical objects discussed in this chapter, they are handled quite differently. The hydrogen bond function searches a displayed structure for possible hydrogen bonds and monitors the interaction of a molecular structure with a substrate. In the QUANTA **Calculate** menu, **Hydrogen Bond** calculates and displays hydrogen bonds any time the structure is changed.

References

1. M. Carson and C. E. Bugg, *J. Molec. Graphics* **4**, 121 (1986).

2. P. Evans, *Daresbury Laboratory Information Quarterly for Protein Crystallography*, 19 (1987).
3. M. L. Connolly, *Science* **221** 709 (1983).
4. P. K. Weiner et al., *Proc. Nat. Acad. Sci US* **79**, 3754 (1982).
5. E. N. Baker and R. E. Hubbard, "Hydrogen bonding in globular proteins" *Prog. Biophys. Molec. Biol.* **44**, 97-197 (1984).
6. C. Giessner-Prettre and A. Pullman, *Theoret. Chim. Acta*, **25** 83-88 (1972).

7. Generating Visual Representations

This chapter describes several mechanisms for displaying and studying structures as solid models. Read this chapter to become familiar with the options for visual representation of your structures.

Some of the visual representations can be manipulated as objects in QUANTA (solid models), some are for display purposes only (raster and raytrace images), and some can be printed as hardcopy (artist plots).

Rendering solid models

Solid Models in the **Draw** menu of the main menu bar provides a number of rendering styles for creating space-filling models. Depending on your workstation, you can display solid models in the viewing area of the Molecule window or in a separate Solid Model window that opens when you make a solid model selection. Displaying solid models in the viewing area requires RGB graphics. Machines with color map graphics use the Solid Model window. The interface for generating solid models is the same for both display mechanisms.

Solid models generated in the viewing area are treated as graphical objects. When a solid model is selected, the Object Management Table is displayed, listing the model as an object. Only one solid model object can be applied to a structure at a time, but several objects (with different names) can be simultaneously displayed.

Different rendering styles can be used in different parts of the structure. Different rendering styles also can be applied to different structures displayed at the same time, but stored in separate MSFs. For more general information about manipulating and displaying graphical objects, see Chapter 6.

The rendering styles available in the **Solid Models** pull-right menu include:

- Ball and stick figures
- van der Waals figures.
- Liquorice models.
- Cartoon models.

Table 35 lists and briefly describes all the selections on the **Solid Models** pull-right menu.

Table 35. Solid Models pull-right menu

Selection	Description
Selection Tools	Opens the Solid Display and Solid Schemes and Utilities palettes.
Protein Cartoon	Generates a schematic model for proteins. Protein molecules must have secondary structures defined.
Van der Waals Spheres	Generates a model where atoms are represented by spheres with radii proportional to the van der Waals radius listed for the atom type in the parameter file that is automatically read in at the start of each Quanta session.
Ball and Stick	Generates a model where atoms are represented by spheres and bonds by cylinders. The radius of the sphere is defined by the plotting radius listed for that atom type in the parameter file that is automatically read in at the start of each Quanta session. The bond thickness is defined by the thin bond specification also contained in the dialog box.
Liquorice Bonds	Generates a model where bonds are represented by cylinders, with the thickness defined by the thickness of liquorice bonds specification (also contained in this dialog box).
Redraw Model	Redraws model with any changes applied.
Settings	Opens a dialog box allowing solid model parameters to be changed. Same as the Parameters selection in the Solid Schemes and Utilities palette.
Translucency	Opens a dialog box for setting translucency of solid models.

Additional modeling choices are available in the Solid Schemes and Utilities palette, opened when you select **Selection Tools** from the **Solid Models** pull-right menu. The Solid Display palette is also opened. Tables 36 and 37 list the selections on these palettes and provide a brief description of each.

Table 36. Solid Display palette

Selection	Description
All MSFs	Display selections affect all MSFs listed in the Molecule Management Table.
One MSF...	Display selections affect specified atoms contained in the specified MSF.
Apply to All MSFs	Copies selection commands to all active structures.
All Atoms	Selects all atoms in the structure.
All Non-hydrogen Atoms	Selects only the nonhydrogen atoms in the structure.
Solvent	Selects all residues of type: WAT, HOH, TIP, TIP3, SOL, SOLV, ST2, NON, H2O, TIP4.
Alpha-Carbon Atoms	Selects only protein alpha-carbon atoms.

Table 36. Solid Display palette (Continued)

Selection	Description
Protein Backbone	Selects only protein backbone atoms.
Protein Sidechain	Selects only protein sidechain atoms.
Nucleic Acid Backbone	Selects only nucleic acid backbone atoms.
Nucleic Acid Sidechain	Selects only nucleic acid sidechain atoms.
Residue Range...	A residue range is selected for display by completing information in a dialog box. The selection process may be repeated.
Residue Types...	Residue types are selected for display by completing information in a dialog box. The selection process may be repeated.
Atom Types	Atom types are selected for display by completing information in a dialog box. The selection process may be repeated.
Pick Molecule	One molecular structure is picked for display using the mouse
Pick Segment	A segment in a molecular structure is picked using the mouse. All atoms in the segment are selected for display. The process may be repeated.
Pick Residue	A residue in a molecular structure is picked using the mouse. The atoms are selected for display. The selection process may be repeated.
Pick Residue Range	A residue range is picked using the mouse. All atoms in the range are selected for display.
Pick Atom	An atom in a molecular structure is picked using the mouse. The selection process may be repeated.
Proximity Tools	Opens the Proximity Tools palette, which has selections for displaying nearby portions of a structure.
Type in a Selection	Selection commands for picking portions of a structure can be typed into a dialog box.
Undo	Returns the display selection to the state before the previous selection.
Clear	Deletes all selections.
Revert	Returns the display selection to the state when the function was first entered.
Quit	Returns the display to the atoms contained in the original selection, and exits the palette without saving.
Finish	Displays the atoms contained in the new selection, and exits the palette.

Manipulating solid models

When a solid model is displayed in the QUANTA viewing area, the model can be manipulated using the techniques that you use for any structure. For example, you can perform global transformations using dials on the Dial Emulator or the mouse and keyboard.

Table 37. Solid Schemes and Utilities palette

Selection	Description
Nothing	No solid model is selected or applied.
Stick	Renders subsequently selected atoms using a stick model. Standard default display
Ball and Stick	Renders subsequently selected atoms using a color-coded ball and stick model.
Liquorice	Renders subsequently selected atoms using a liquorice model.
VDW	Renders subsequently selected atoms as spheres with radii proportional to the van der Waals radii in the atom type parameter file.
Sheet	Renders subsequently selected atoms in a protein using a thick ribbon model of protein backbone.
Ribbon	Renders a designated portion of a molecule using a thin ribbon model.
Helix	Renders a helical portion of a molecule using a thick ribbon model.
Cylinder	Displays a cylinder through the helical portion of a molecule
Secondary Structure	Applies secondary structure to a protein molecule.
Parameters	Opens a dialog box allowing changes in solid model parameters. Same as Settings selections in the Solid Model menu.
Translucency	Opens a dialog box for setting translucency of solid models.
File and Edit Options	
Read Selection Commands	Reads commands from file.ssd and updates the viewing area to reflect the new set of commands.
Append Selection Commands	Appends the current .sol with a set of commands from another file, file.ssd f and updates the viewing area to reflect the new combined set of commands.
Save Selection Commands	Saves the current set of commands to a new file.ssd. Only available when One MSF is selected in the Display Atoms palette. Selections can be saved for only one MSF at a time.
List Selection Commands	Displays the current selection commands in the textport.
Edit File Manually	Allows a .dsf file to be manually edited. A new window is opened which uses the vi editor for editing the file ^a .
Help on Commands	Provides a list in the textport of display selection commands that can be used from the keyboard. Each entry includes a short example.

^aYou can change the default editor by using the UNIX `setenv` command before QUANTA is started. The syntax is: **setenv EDITOR name_of_text_editor**.

When you move a structure to which you have attached an object, the object, by default, is hidden during the movement. This helps speed up manipulation, particularly of complex molecules.

If you want the object to be visible throughout the manipulation, open the **Preferences** menu, select **Suppress Objects**, then select **Off** from the pull-right menu that opens. All objects will be displayed during movement of the structure until you change the preference.

Using the Solid Model window

Solid model display in the viewing area requires that a machine use RGB graphics. Machines with color map graphics use the Solid Model window. The interface for generating solid models is essentially the same for both display mechanisms. The difference is that with machines using the Solid Model window, solid model graphical objects are displayed in this window, not as an integrated display in the Molecule window.

If your machine uses the Solid Model window, models are manipulated by placing the cursor in the window and using standard cursor–keyboard combinations for translation and rotation. Structures containing more than 15 atoms may require a considerable period of time to redraw in the new orientation.

The size and position of the Solid Model window can be changed using the standard workstation window manager. When a window is open, the left mouse button can be used to display a popup for modifying various aspects of the solid model display. Selections are made from this menu (and other menus called by this menu) by using the *right* mouse button.

Table 38 lists and briefly describes the selections in this popup. Tables 39 and 40 list and describe the selections in submenus of the Solid Model window popup.

Table 38. Solid Model Window menu

Selection	Description
Settings	Defines the model image sharpness, from Rough and Ready (coarser image-fastest screen rewrite) to Maximum (highest resolution, slowest screen redrawing).
Spheres	Defines the tessellation level for spheres (2–20).
Cylinders	Defines the number of polygons in bond cylinders (5–100).
Ribbons	Defines the number of interpolation points for each residue (2–20).
Full Screen	Enlarges the Solid Model window to fill the monitor screen.
Stereo	Opens a dialog box to set parameters for the stereo image.

Table 38. Solid Model Window menu (Continued)

Selection	Description
Reset View	Resets the view to the original view when the solid model was started or to the last saved view if a view was saved.
Save View	Saves the current view.
Title On	Displays the mouse instruction for displaying the Solid Modeling menu (in the lower-left corner of the Solid Modeling window).
Title Off	Erases the mouse instruction for displaying the Solid Modeling menu.
Exit	Exit Solid Modeling and return to Quanta.

Table 39. Solid Model Window stereo selections

Selection	Description
Stereo Off	Turns stereo off.
Internal Stereo	Displays two views of the structure, one above the other, for use with SGI's Stereo View hardware to view stereoscopic images.
External Stereo	Displays two views of the structure, one above the other, for use with SGI's stereoscopic display to view stereoscopic images.
Side-by-Side	Displays both views of the stereo pair side by side within the molecule window.

Table 40. Solid Model Window settings selections

Selection	Description
Rough 'n' Ready	Sets model resolution to coarsest setting and fastest redraw.
Reasonable	Sets model resolution to a finer setting than Rough 'n' Ready .
Very Good	Sets model resolution to an even finer setting than Reasonable .

Sample procedure — Generating a solid model

Complete the following exercise to become familiar with creating and modifying solid models. This exercise uses the structure mypeptide, built in the *Creating a Peptide* section of Chapter 4. It assumes you are working on a workstation with RGB graphics.

1. Open mypeptide.msf.

Display the **File** menu and select the **Open** function. Select mypeptide.msf from the File Librarian dialog box scrolling list. Select the **Replace** option and then the **Open** button.

2. Choose a solid model to display.

Display the Draw menu and select **Solid Models**. From the pull-right menu that opens, select **Ball and Stick**. The structure mypeptide is displayed in the viewing area using the ball and stick model. The Object Management Table is displayed listing the object SOL_object.

3. Select another solid model rendering.

Display the **Draw** menu again. Select **Solid Models** and then select **Liquorice** from the pull-right menu. The mypeptide structure changes to a liquorice model. There is no change in the Object Management Table.

Select the **Displayed** column for SOL_object. The text changes from yes to no, and the structure returns to the standard stick display.

Select the **Displayed** column again. The text changes from **no** to **yes**, and the liquorice model is displayed again.

4. Change solid model settings.

In the Modeling palette, select **Hydrogen Bonds**

From the **Draw** menu, select **Solid Models**, and then select **Settings** from the pull-right menu. In the dialog box that opens, enter the value:

Thickness of Liquorice Models: 0.4

Select the option:

Solid Hbonds On

Enter the value:

Hbond Thickness: 0.2

Select the **Redraw** button and the display changes to reflect the changes you have made.

Return to the **Draw** menu, select **Solid Models**, and then select **Ball and Stick** from the pull-right menu. The Object Management Table remains unchanged.

5. Apply Selection Tools.

From the **Draw** menu, select **Solid Models**, and then select **Selection Tools** from the pull-right menu. The Object Management Table is removed, and the Solid Display and Solid Schemes and Utilities palettes are opened.

In the upper-right corner of the viewing area, modeling choices are presented in a color-coded list, which duplicates the choices in the Solid Schemes and Utilities palette.

The molecule display changes to a red stick model. (The red color indicates the **Ball and Stick** model has been selected.) In the viewing area list, **Ball and Stick** is marked with a *, and **Ball and Stick** is checked and highlighted in the Solid Schemes and Utilities palette. No model is actually displayed until you exit Selection Tools.

6. Clear all solid models.

Select **Clear** from the Solid Display palette and **Nothing** from the Solid Schemes and Utilities palette. Nothing is checked and highlighted and the structure turns pale green.

7. Select several solid renderings for different parts of the structure.

From the list in the upper-right corner of the viewing area, select **Ribbon**. **Thin Ribbon** is checked and highlighted in the Solid Schemes and Utilities palette.

In the Solid Display palette, select **Protein Backbone** and the structure's protein backbone is displayed in purple.

From the list in the upper-right corner, select **VDW Spheres**.

From the Solid Display palette, select **Pick Residue** and the message line reads:

Select the atoms to be type VDW. Pick atom to select residue.

Pick an atom in the residue of your choice and the residue turns white.

8. Apply your selections.

From the Solid Display palette, select **Finish** and the Selection Tools palettes are closed. The structure is displayed in the viewing area with a pale green ribbon backbone and a single residue modeled as van der Waals spheres. The Object Management Table reopens listing SOL_ object.

9. Delete all solid objects.

Select the **Delete** column of the Object Management Table. The structure returns to a standard stick display and the Object Management Table closes.

Generating cartoons of proteins and nucleic acids

Cartoons can be generated for different types of molecules including proteins and nucleic acids. To generate a cartoon from a protein file, the secondary structure must be defined. If you have a protein without a defined secondary structure, use the Protein Design application in the **Applications** menu to define the structure before you generate a cartoon solid model.

Complete the following exercise to become familiar with creating protein and DNA cartoons. This exercise uses the structures `complex_dna` and `complex_prot`. To copy the MSFs into your QUANTA tutorial directory, issue this UNIX command while in that directory:

```
> cp $QNT_ROOT/userguide/complex_*.msf .
```

The structures represent a modeled interaction of a modified DNA with a protein. `Complex_prot.msf` already contains secondary structure information for the molecule.

1. Open `complex_prot.msf` and `complex_dna.msf`.

From the **File** menu, select **Open** and a File Librarian dialog box opens.

From the dialog box scrolling list, select `complex_prot.msf` and then `complex_dna.msf`.

Select the **Replace** option and then click the **Open** button.

2. Apply Solid Selection Tools.

From the **Draw** menu, select **Solid Models**. From the pull-right menu that is displayed, select **Selection Tools**. The Solid Display and the Solid Schemes and Utilities palettes are displayed.

3. Set up protein cartoon parameters.

From the Solid Display palette, select **One MSF...** and a dialog box opens. From the dialog box scrolling list, select `complex_prot.msf`.

From the Solid Schemes and Utilities palette, select **Parameters...** In the Solid Models Settings dialog box that opens, click the **Reset to**

7. Generating Visual Representations

Default Values button. This sets the appropriate parameters for protein cartoon drawing.

If you want alpha helices to be drawn as cylinders, check the **Draw Helices as Cylinders** option, and then click the **OK** button.

4. Select the protein cartoon.

From the Solid Schemes and Utilities palette, select **Secondary Structure**.

Then from the Solid Display palette, select **All Atoms**. The protein backbone is colored to show the zones that are sheet, ribbon, helix, or cylinder.

5. Set up DNA cartoon parameters.

Select **One MSF...** from the Solid Display palette and a dialog box opens.

From the dialog box scrolling list, select `complex_dna.msf`.

From the Solid Schemes and Utilities palette, select **Parameters...** and the Solid Models Settings dialog box opens.

Enter these values to optimize the settings for DNA display:

Atom defining path of ribbon: C1'

Maximum Distance Apart of Atoms: 7.0

Offset of ribbon from guide atom: 1.

Helix Thickness: 0.8

Ribbon Width: 0.6 Thickness: 0.6

Select:

Draw “rungs” between double-helix “ladders”

Click the **OK** button.

6. Select the DNA cartoon.

From the Solid Schemes and Utilities palette, select **Helical Ribbon**.

From the Solid Schemes and Utilities palette, select **All Atoms** and the C1' guide atoms are displayed in purple.

7. Display the cartoon.

From the Solid Display palette, select **Finish** and a solid model graphical object is displayed for each MSF. Ribbons are colored according to the color of the guide atoms, in this case, the default color, light green.

The Object Management Table is displayed, listing an object for each structure.

8. Change the color scheme.

From the **Draw** menu, select **Color Atoms**. Then from the pull-right menu that is displayed, select **Selection Tools**. The Color Schemes and Utilities and the Color Atoms palettes are displayed.

From the Color Schemes and Utilities palette, select **Color by Secondary Structure**.

From the Color Atoms palette, select **Pick Segment**, and then pick an atom in one of the DNA chains.

From the Color Atoms palette, select **Next Color Number**, and then pick an atom in the other DNA chain.

9. Display the cartoons with the new color scheme.

From the Color Atoms palette, select **Finish**. The protein should now be colored according to the secondary structure, with the DNA chains blue and red.

From the **Draw** menu select **Solid Models**. From the pull-right menu that is displayed, select **Redraw Model**, and the solid models are re-created using the new color scheme.

10. Display the solid models only.

To show just the solid models without the usual vector bond display, open the **Draw** menu and select **Manage Display**.

From the dialog box that opens, toggle **Bonds** off. Then click the **OK** button.

To restore the display of bonds, press the <F10> key.

11. Return the structures to their original display.

In the Object Management Table, select the **Delete** cell for each object and the objects are removed from the viewing area.

7. Generating Visual Representations

From the **Draw** menu, select **Color Atoms**, and then select **By Element** from the pull-right menu that is displayed. The structures are colored by element.

Generating solid surfaces

The **Solid Surfaces** item on the **Calculate** menu offers the following choices on the pull-right submenu:

Calculate]Calculates a solid surface for each currently displayed MSF using the current settings and displays the surface. Each surface occupies a graphical object, so their display can be toggled or they can be deleted using the Object Management table in the usual way. (For more information about the Object Management table, see *QUANTA: Generating and Displaying Molecules*, Chapter 6.) The surface objects are named SUR_*msfname*. To create an alternative surface for an MSF while keeping an existing one, click its name in the Object Management table and change its name from this default.

The surface calculation can be aborted before completion by clicking the mouse.

Options Displays a dialog box giving the options for calculating and displaying solid surfaces. The options are:

- Use a fixed grid mesh size or calculate the grid size so that there is some maximum number of grid points along one side. The fixed size parameter, in that case, is used as the minimum value.
- The surface can be calculated either as some percentage of the van der Waals radii of the atoms or as the van der Waals radii plus a probe radius.
- Coloring options are: **By Atom**; **Electrostatic**; **By Molecule**; or **All** in one specified color.
- Translucency: Four settings, ranging from opaque to transparent.
- Whether to save the surface to a file so that it can be re-displayed or plotted subsequently. The surfaces can be retained indefinitely or until its MSF is closed. The surface files will be called *msfname_calc.tri*.

If you choose to proceed with the calculation rather than just setting the preferences, it will be displayed after calculation and the display adjustment palette will be entered (see below). This allows alteration of the surface display even if it hasn't been saved to file.

<i>Color as Nearest Atom</i>	Re-Display If you opted to save surface files, the surface can be recreated in different styles. A palette is displayed with the following tools: Each vertex is colored like the nearest atom.
<i>Color by Molecule</i>	The surface for each MSF is colored differently.
<i>Color by Electrostatics</i>	The electrostatic potential at the surface is calculated, using the current atomic charges. A dialog box appears that allows you to control the energy range and color numbers for the color ramping.
<i>Re-bin Electrostatics</i>	Allows you to re-display the electrostatic surface with different ramping without recalculating it.
<i>Tonal Color Ramp</i>	Displays a dialog box that allows control of the tonal color ramping (for example, the blue to red to white that is used for electrostatics).
<i>Spectral Color Ramp</i>	Displays a dialog box that allows you to control the spectral color ramping (for example, red to blue to green).
<i>Default Colors</i>	Resets the color values to default settings.
<i>Opaque</i>	Make the surface opaque. Nearly Opaque Make the surface nearly opaque.
<i>Nearly Translucent</i>	Make the surface nearly translucent.
<i>Translucent</i>	Make the surface translucent.
<i>Finish</i>	Exit the palette.
<i>Preferences/All Settings/ Solid Patterns (command SET PATT)</i>	Related commands The quality of the solid surface representation depends on the graphics hardware. Even with base-level graphics, you can improve the display using the following options: Toggles between two alternative pattern sets to be used for the semi-opaque surfaces.
<i>Command VIEW SINGLE ON/OFF</i>	Sets the system to single-buffer mode when the molecule is stationary. This allows all the available bitplanes to be used for rendering the picture. Double-buffer mode is resumed when the molecule starts to move. Inevitably, you will see the picture being redrawn in between, so this option is not recommended for normal use, rather it should be turned on prior to taking photos, etc., and turned off afterwards.
<i>Command SET BACK ON/OFF</i>	Turns on or off backface polygon removal for the solid surface. This has the effect of removing any polygons for which the face (normal) of the polygon is facing away from the viewer. This has the effect of additional clipping, allowing buried molecular surfaces to be clipped for viewing purposes.

Generating raytrace van der Waals models

Raytrace is a pull-right menu in the **Draw** menu that contains several options for creating a pseudo-3D rendering of structures displayed in the workspace. The rendering employs both highlight and shadow detail to provide a better defined image. Ray-traced movies can be scripted.

Original Raytrace This option executes the original raytrace program that has been available with QUANTA for many years, which produces an image of a van der Waals representation of the currently displayed atoms.

1. Display the 3D rendering of a structure.

Display the Draw menu and select **Raytrace/Original Raytrace**. A ray-traced image of a van der Waals representation of mypeptide.ms is generated in the Ray Tracing window.

2. Remove the rendering and return to original display.

With the cursor is in the Ray Tracing window, click the left mouse button and the Ray Tracing window closes.

Rayshade Solid This option executes the Rayshade program (see below) to produce a ray-traced image of the currently displayed solid graphics objects (e.g. van der Waals, protein cartoon, or solid surfaces). QUANTA generates an intermediate file called run.rayshade containing commands and graphics primitives for the rayshade program. This is run and the output placed in a file called r.rle. The RLE file can be viewed using the Utah Raster Toolkit.

On requesting a Rayshade Solid drawing, a dialogue box is displayed which prompts for the size of the image to be produced and whether a background plane is to be included in the image. Images of 300 pixels should be generated to start with, since generation can take considerable time.

The Rayshade program is in the public domain and can be obtained over the internet from several sites. Contact your Accelrys support office for information on how to obtain the program.

Generating display-only raster models

The **Raster Models** selection in the **Draw** menu generates space-filling representations of a displayed structure. When **Raster Models** is selected, a pull-right menu opens with selections for the style of raster model to be displayed. Table 41 lists the selections and provides a brief description of each.

Table 41. Raster Models pull-right menu

For all options, the displayed disks or spheres represent atoms and are colored according to the current color selection.

Selection	Description
Z-buffered Spheres	Generates CPK representation of the structure using correctly intersecting and smooth-shaded spheres. Available only on workstations with z-buffering hardware.
Flat Disk	Generates colored disks.
Outlined Disk	Generates colored disks outlined in black.
Smooth Spheres	Generates shaded spheres.
Metallic Spheres	Generates shaded spheres with a metallic hue.
Interpenetrating Spheres	Generates interpenetrating spheres. If z-buffering is on, individual atoms are drawn in the order they are displayed in the z plane. If z-buffering is off, individual atoms are drawn in the order they are listed in the MSF.

The representations are for display purposes only. Representations cannot be rotated or interrogated, but can be printed if the workstation is equipped with an output device capable of accepting screen dumps or photography.

Plots for hardcopy output

The **Plot Molecules** menu in the **File** menu is used to define and create plot files for the generation of hard copies of structures. The plots can be previewed on the screen before hardcopies are generated.

The types of output files are:

Artist Plots

Uses an external program to produce ball and stick, van der Waals, or user-defined representations of structures for publication quality plots. The **User-defined** option offers a list of commands that define how the structure(s) can be rendered.

7. Generating Visual Representations

<i>Stick Plots</i>	Creates a plot of the molecule using the currently stored information about bonds, labels, IDs, hydrogen bonds, and other pertinent parameters. Graphic objects are not plotted in this mode.
<i>Molecular Graphics View Plot</i>	Creates a plot of all the currently displayed vector, dot, and text information in the graphics window. The image is clipped as seen on the screen. This option is only available on Silicon Graphics workstations that support the feedback buffer mechanism used.
<i>MolScript Plots</i>	Creates high-quality hardcopy output of molecular structures including protein cartoons.
<i>Color Screen Images</i>	Available only on certain Silicon Graphics workstations, creates an image file of the current screen and converts the image to PostScript format. The UNIX programs scrsave, iflip, and tops must be in your path.
<i>Solid Plots</i>	Creates a PostScript plot of any solid models or surfaces. The first five of these plottypes are created by selecting Generate from the Plot Molecules menu. Table 42 lists the plot options available in the Setup Hard Copy Plot of Molecules dialog box.

Table 42. Hard Copy Plot options

Option	Description
Plot type	
Artist Plot	Creates plot using the Artist program, in one of the following three styles. The output is a QUANTA plot format file which can be further processed.
Ball and Stick	Renders a molecule using the ball and stick model.
Van der Waals	Renders a molecule using atoms represented by spheres with radii proportional to the van der Waals radii in the parameter file.
User Defined	Renders a molecule using a user-defined model. Opens a dialog box that allows you to specify the model.
Stick Plot	Renders a molecule using stick plot model.
Molecular Graphics View	Renders the current vector, dot, and text objects in a QUANTA plot format file for further processing.
MolScript Plot	Uses the third-party program MolScript to create a high quality PostScript plot of the molecules, including solid models.
Color Screen Image	Uses the GL scrsave utility to create an image file of the current screen and converts the image to PostScript format; SGI machines only — scrsave, iflip, and tops must be in your path.
<i>View To Use (not applicable to all types of plot)</i>	
Current View	Renders a molecule using the current view.

Table 42. Hard Copy Plot options

Option	Description
From View File	Calls a File Librarian that allows you to select a view file to define the molecule's orientation for the plot file.
Identify Matrix	Plots the molecule in the orientation that is stored in the MSF.
Plot Scale (mm/Å)	Calculates the scale automatically for the plot to fill the page. Can be modified.
Plot Titles and Borders	Generates the plot file containing title and border.
Title	Allows you to enter a title for the plot.

The **MolScript** and **Color Screen Image** create PostScript plot files directly. These may be previewed using the **Preview** selection in the **Plot Molecules** menu; the function automatically detects if the file is in PostScript format and if so uses the xpsview program instead of the usual QUANTA preview program.

The other plot types first produce a QUANTA plot file, which is a general-purpose binary file containing graphical information. (Please see Appendix C in the *Basic Operations* guide for further details). A dialog box is then displayed giving a choice of plot disposition options.

You can also use the Preview selection in the **Plot Molecules** pull-right menu (under the **File** menu) to view the contents of a QUANTA plot file on the screen. Or you can use an interactive figure editor in the user_group_ files area to convert the file to a format accepted by the xfig program distributed by Silicon Graphics.

Table 43 lists and briefly describes the options in the Plot Disposition dialog box.

Table 43 Plot Disposition options

Option	Output Type
Preview Plot	Renders a structure in the QUANTA Preview window approximating the hardcopy appearance.
Regenerate Plot	Returns to the Setup Hard Copy dialog box, to modify the plot characteristics.
HPGL Format	Creates an output file in a format compatible with Hewlett-Packard plotters or other devices that are HPGL compatible.

Table 43 Plot Disposition options (Continued)

Option	Output Type
Color Idraw	Creates an output file in idraw format.
B&W Idraw	Creates an output file in idraw format, converted to black and white
Color PostScript	Inserts RGB color values for each colored object. Color is only visible on color PostScript output devices.
B&W PostScript	Creates a black and white PostScript file
QUANTA Plot File	Saves a QUANTA plot file.

Producing a hardcopy plot is a two-stage process. The first stage involves specifying the type of plot required. The second stage involves specifying how the plot is to be output.

Complete the following exercise to become familiar with the procedure for producing hardcopy plot.

1. Produce a ball and stick artist plot with a scale of 5 mm per angstrom.

Display the File menu and select **Plot Molecules**. From the pull-right menu that opens, select **Generate**. In the Setup Hard Copy Plot of Molecules dialog box that opens:

Select the options:

Artist Plot
Ball and Stick
Current View

Enter the value:

Plot Scale (mm/Å):5.0

Select the option:

Plot Titles and Borders

Enter the text:

Title: mypeptide

Click the **OK** button. After a short wait, the Plot Disposition dialog box offers options for viewing and printing the plot.

Select the option:

Preview Plot

Click the **OK** button and the ball and stick rendered peptide molecule is displayed in the QUANTA Preview window. Information about the rendering is displayed at the bottom of the window.

Move the cursor inside the QUANTA Preview window and click the left mouse button. The window is removed from the screen and the Plot Disposition dialog box opens.

At this point, you can return to the **Setup Hard Copy Plot** option in the Molecules dialog box to alter the appearance of the plot. If you do so, select the **Regenerate Plot** option after making your changes. Or you may create output of the plot displayed on the screen.

2. Create a PostScript File using ball and stick rendered peptide.

From the Plot Disposition dialog box, select the options:

PostScript Format

Translate as Color and Texture (under PostScript options)

Click the **OK** button and a File Librarian dialog box opens.

Enter the text mypeptide and click the **Save** button to save the PostScript file as mypeptide.ps. The file is created and you are returned to Molecular Modeling mode.

3. Output hard copy of a PostScript (.ps) file.

The procedure for sending the .ps file to a particular PostScript output device depends on how the computer is set up, network hardware and software being used, and the output device. Please consult with your system administrators.

4. Generate a user-defined output file.

Display the **File** menu and select **Plot Molecules**. In the Setup Hard-copy Plot of Molecules dialog box that opens, select the option:

User Defined

Click the **OK** button and a dialog box opens to accept commands specifying how the structure is rendered.

Enter the text **Help** in the data entry field to view a list of available commands in the textport. These commands, their form, and a brief description of each are listed in Table 44.

7. Generating Visual Representations

Table 44. Artist Plot user-defined commands

Com-mand	Form	Description
Bond	BOND <i>type</i> <i>col sel</i>	Defines the color (<i>col</i>) and drawing style of bonds (<i>type</i>) associated with the atoms identified with the atom selection command (<i>sel</i>). For example, BOND 1 1 sele zone 1 to 21 specifies the bonds in residues 1 to 21 are drawn with bond type 1 using color number 1.
Color	COLO <i>col</i> <i>sel</i>	Defines the color (<i>col</i>) for atoms identified with the atom selection command (<i>sel</i>). For example, COLO 7 sele pick n specifies all nitrogen atoms are drawn in color number 7.
Define	DEFI <i>type</i> <i>thick</i> <i>vector</i>	Defines the style of bonds (<i>type</i>), the thickness of the bond in angstroms (<i>thick</i>), and the number of vectors (<i>vector</i>) used to create each bond. For example, DEFI 2 0.05 5 defines vector thickness of 0.05 Å represented by 5 lines for bond type 2.
Radius	RADI <i>rad</i> <i>sel</i>	Defines the radius of the sphere in angstroms (<i>rad</i>) used to represent the atoms identified with the atom selection command (<i>sel</i>). For example, RADI 1.0 sele pick h draws hydrogen atoms using a radius of 1 Å.
Shade	SHAD ON <i>ang1</i> <i>ang2 sel</i>	Defines the direction of rotation for shading from the x and y planes (<i>ang</i> , <i>ang2</i>) for atoms identified with atom selection command (<i>sel</i>). For example, SHAD 90 0 sel pick CA end specifies that alpha carbons are shaded and the vector representing the shading is drawn at 90°. SHAD NONE sele all specifies no atoms are shaded.
	SHADE OFF <i>sel</i>	Turns shading off.
Set Radius	SRAD <i>sel</i>	Defines plotting radius of the spheres for atoms identified with atom selection command (<i>sel</i>).
van der Waals	VDW% <i>sel</i>	Defines the percentage (%) of the van der Waals radius for atoms identified with the atom selection command (<i>sel</i>). For example, VDW 50 sele pick CA N C O end specifies the mainchain atoms of a protein are drawn at a radius of 50% of their van der Waals radii.
Draw	DRAW	Generates the plot.

MolScript plots

MolScript is a program for creating molecular graphics in the form of PostScript plot files. Possible representations are simple wire models, CPK spheres, ball-and-stick models, text labels, and Jane Richardson-type schematic drawings of proteins, based on atomic coordinates in various formats. Color, grayscale, shading, and depth cueing can be applied to the various graphical objects.

The QUANTA interface to MolScript generates the input script and coordinate files to reproduce as nearly as possible the current representation. Objects rendered include bonds, solid models, hydrogen bonds, distance monitors, labels, and atom IDs.

Quanta supports several versions of Molscript that have a few differences in capability and keywords. Please make sure you fill in the correct version number in the MolScript options dialog.

The interface is accessed by using the function **Plot Molecules** → **Generate** on the **File** menu. This displays the usual Setup Hard Copy Plot of Molecules dialog box, which includes a **MolScript Plot** radio button. When this is used, a dialog box is displayed containing the MolScript interface options.

Version Number Specifies which version of Molscript you have installed.

Root name for files The interface produces two files, *filename.pdb* containing the molecular coordinates, and *filename.in* containing the MolScript commands. Running the program produces the PostScript file *filename.ps* or *filename.eps*.

Maximum bond distance This is used to control the maximum bond distance allowed in ball-and-stick plots. The default 2.1 Å is suitable for proteins containing disulfide bridges but no hydrogen atoms; if hydrogen atoms are present, a smaller value is needed to prevent the hydrogen atoms from being bonded together. Vector bonds are generated using the **LINE** command, so that the exact bonding generated by QUANTA can be replicated regardless of this setting.

Draw thin ribbons as turn or coil MolScript allows for optional smoothing of thin ribbons. This can make for a clearer diagram, but should be avoided if sidechains are also displayed.

Thin ribbon all one color This can sometimes make for a clearer diagram.

Change to solid color scheme Changes the color settings to be optimized for the drawing of solid models. The plot always has a white background regardless of the QUANTA background color.

Retain input MolScript and pdb files Allows the input files to be retained — expert users may want to manually adjust the input and rerun MolScript. If this option is unchecked, then the input files will be deleted if MolScript is run successfully.

Preview plot This option causes the resulting PostScript plot to be displayed with the xpsview viewing program. Xpsview or an alias pointing to it must be in your path.

7. Generating Visual Representations

If both solid models and vector bonds are displayed on screen, then both are included in the MolScript plot. Remember that vector bonds can be rapidly toggled using function key <F10> if the default key bindings are set up. Otherwise, enter the commands **HIDE BOND** and **SHOW BOND**.

When the **OK** button is clicked, the input files are created and MolScript is run.

To obtain MolScript

The MolScript program must be obtained from its author, Dr. Per Kraulis.

Per Kraulis, Ph.D phone: +46 (8) 695 78 34
Pharmacia & Upjohn, Inc. fax: +46 (8) 695 40 82
PPC Sweden Research, N62:5e-mail:
S-112 87 Stockholm krp@sgirpe.sto.se, pn@pn.se
SWEDEN or p.j.kraulis@bioc.cam.ac.uk
or molscript@bioc.cam.ac.uk

The software is provided under license — details from Per Kraulis.

In publications, you must refer to:

Per J. Kraulis “MOLSCRIPT: a program to produce both detailed and schematic plots of protein structures” *J. Appl. Crystallog.* **24** 946–950 (1991).

Summary

This chapter describes several mechanisms for visually representing structures. Some of the visual representations can be manipulated as objects in QUANTA (solid models), some are for display purposes only (raster and raytrace images), and some can be printed as hardcopy (artist plots).

The **Solid Models** function in the **Draw** menu provides several styles for rendering space-filling models. Depending on your workstation, solid models are displayed in the viewing area of the Molecule window or in a separate Solid Model window.

Solid models generated in the viewing area are treated as graphical objects. Only one solid model object can be applied to a structure at a time, but different rendering styles can be used in different parts of the structure. Different rendering styles also can be applied to different structures displayed at the same time but stored in separate MSFs.

The rendering styles available in the **Solid Models** pull-right menu include: ball and stick, van der Waals, licorice, and cartoon models.

Raytrace in the **Draw** menu is a selection that creates a pseudo-3D rendering of structures. The rendering employs a van der Waals model and uses

the default atom sizes and colors that are set up before Raytrace is selected. It employs both highlight and shadow detail to provide a better defined image. The image cannot be manipulated.

The **Raster Models** selection in the **Draw** menu also generates space-filling representations of a displayed structure. The representations are for display purposes only.

The **Plots** selection in the **File** menu is used to define and create plot files for generating hard copies of structures. The plots can be previewed on the screen before hardcopies are generated.

7. Generating Visual Representations

8. Importing and Exporting Files

Molecular structures are held in various applications. The files containing data on these structures use formats that are different from the MSF format. The **Import** and **Export** functions in the **File** menu allow you to read and write external file formats to and from QUANTA. Imported files usually require a certain amount of processing before they can be used in calculations such as CHARMM energy calculations. This can be done using the **Split and Clean** function.

The **Import** function allows an external file format to be read into QUANTA, creating an MSF and displaying its associated structure. The MSF is assigned the same name as the external file, and QUANTA automatically adds the extension .msf. An external file format can also be read into the MSF of a structure that is currently displayed.

The **Export** function reverses the import process, allowing structures in MSFs to be converted to the appropriate format and read into an external database.

The **Split and Clean** function on the **Edit** menu facilitates adding hydrogens and assigning atom types and bond orders using tools appropriate to various classes of molecules.

Formats that can be handled by QUANTA include:

- Protein Data Bank.
- CNX/X_PLOR/CHARMM PDB.
- CHARMM CRD.
- CHARMM PSF and CRD.
- ChemNote.
- QM Coordinate.
- BioDesign BGF.
- MDL 2D/3D.
- Cambridge FDAT.
- Fractional Coordinates.
- Gromos.

Although a standard process is used to create an MSF, the actual steps may vary depending on the format that is selected. Selection criteria may be manually or automatically specified at the time the MSF is created.

Importing PDB files

PDB import/export preferences

Several conditions may require special handling when a PDB file is imported. If this happens, QUANTA displays a dialog box asking you to choose what should be done. For example, if the crystallographic space-group is missing, QUANTA asks you to confirm that it is. Or, in the Brookhaven standard format, a character in column 17 is an alternate position indicator, but some programs create “pdb” files treating this field as part of the atom name. So correct interpretation of the data requires you to have some knowledge of the provenance of the file. However, for genuine Protein Data Bank files, the import process can be simplified by turning off some or all of these prompts and assuming that the data is in the standard format. This can be done by selecting **PDB Import/Export** from the **Preferences** menu and turning on some or all the toggles. During subsequent PDB importation, if any of the conditions arise, a message is output to the textport.

Additionally, during both import and export, atoms may need to be renamed to match a format’s conventions. To automatically rename PDB files, display the **Preferences** menu and select **PDB Import/Export**. In the Automatic PDB File Renaming Options dialog box, the standard options for import and export, respectively, are:

Change to QUANTA Standard Names
Change to IUPAC/Brookhaven Names

PDB files containing multiple models

Some PDB files contain multiple conformers — usually as a result of NMR structure determination. By default, QUANTA reads the first conformer and creates an MSF containing this structure. If you turn on the **Prompt for Multi-MODEL options** toggle in the PDB Import/Export Preferences dialog box, then, whenever you import a file containing MODEL records, you are prompted to choose which conformer should be used to create the MSF and also whether to create a .csr file containing the coordinates of all conformers. The .csr file can then be used in the Analysis application.

Importing Protein Data Bank files

To set preferences for multi-model PDB files

You can create an .msf from any single structure in a Protein Data Bank file that contains more than one model. For Protein Data Bank files that contain conformers, you also can create a .csr file to contain all the conformers (see above).

1. Select **PDB Import/Export** from the **Preferences** menu. The Automatic PDB File Renaming Options dialog box is displayed:
2. Check **Prompt for Multi-Model options**, then click **OK**.
3. Select **Import** from the **File** menu. A File Librarian is displayed:
4. Select the file you want to import and the **Protein Data Bank** format (the default selection), then click **Import**. A dialog box with multi-model file options is displayed:
5. Indicate the model number you want to import and check the check box if you want to create a .csr file for all the models in the Protein Data Bank file. Then click **OK**. The file is imported. If there are any non-standard atom types in the file, QUANTA prompts you to choose options for typing the atoms.

The task is now complete.

Importing multiple PDB files

The function **Import Multiple PDBs** on the **File** menu facilitates importing several PDB files at a time. All the prompting described above is suppressed during this operation. A dialog box similar to that used for opening MSFs is displayed, allowing one or more PDB files to be selected. These can be all standard Brookhaven format or all CNX/X-PLOR/CHARMm style. The resulting MSF files can replace any currently open MSF file or be appended to it.

Cleaning imported structures

Structures imported from external sources, for example, Protein Data Bank (PDB) files, frequently need some editing prior to further work within QUANTA. The files may contain a variety of different chemical entities (protein, solvent, nucleic acid, ligands, ions) for which different editing tools are most suited. For instance, amino acids can have names standardized, forcefield types and bonds correctly assigned, and hydrogens added by means of tools in the Protein Design application which uses templates

8. Importing and Exporting Files

for these structures. Ligand molecules within PDB files more often need manual editing to generate correct bonding and atom types; this can be done quickly and easily within the Molecular Editor, especially if the ligand is treated alone rather than as part of the entire protein–ligand complex.

Split and Clean on the **Edit** menu facilitates such operations. It provides a straightforward method for dividing a structure into its constituent parts and the tools necessary for editing each part.

On entering this function, each residue within the structure is automatically classified as protein, solvent, nucleic acid, or other and colored accordingly. You may add extra classifications (e.g., ligand, ions) and can reassign residues or whole segments. A pickable color-coded legend appears in the top right corner of the molecule window.

Splitting tools

Color by Classification This tool toggles between coloring the structure according to the classification of each residue and the normal color selection.

Default Classification This tool can be used to return to the default classifications set by the program.

Classify Separate Segments Operates on residues classified as *other*, making a new classification for each segment.

Classify Picked Residue Before using this tool, click the desired classification from the legend, denoted by a star. When the tool is turned on, you are prompted to click the residue(s) that are to become this type. Clicking the tool again turns it off.

Classify Picked Segment As above, but reclassifies an entire segment.

Classify Residue Type A dialog box is displayed which contains a scrolling list of the residue types within the system. One or more can be selected to be reclassified.

Undo Last Classification Undoes the last change to the residue classifications.

Add Classification Displays a dialog box in which you can indicate the name of an additional classification.

Change Class Names Displays a dialog box containing the editable names of all the existing classifications, each of which must be unique.

Save to Separate MSFs Once residue classification has been performed to your satisfaction, use this tool to create a separate MSF for each classification, the name of which is the original root name followed by an underscore and the class name.

Revert Returns to the original MSF (as it was when the function was first entered).

Cleaning tools

Once the system consists of MSFs, each containing one type of residue (i.e., after the use of **Split and Clean** or immediately, if the function is entered with a set of such structures), the tools that facilitate cleaning the structure are enabled. The file `protein_structure.gsd` holds the definitions used to clean the protein.

Clean Options Displays a dialog box that allows you to choose which hydrogen representation should be applied — **Polar**, **All**, or **None**.

Clean Protein Operates on any active MSFs that consist entirely of residues recognized as amino acids or classified as protein. The clean process includes:

Disorder handling

If the structure contains disordered atoms, gives you the choice of whether to retain them or to keep just one set.

Atom Name standardization

Atom names are changed to conform to the standard amino acid nomenclature as defined in the protein template files (`$HYD_LIB/protein_structure.gsd`).

Termini fixing

Ensures all terminal atoms are present and correct.

Residue completion

If the residue is missing atoms, these are added using the standard amino acid templates, but given an occupancy of zero.

Hydrogen addition/deletion

Hydrogens are added or deleted according to the choice set in the Clean Options dialog

Atom typing

At the end of this operation, the atom types should all be correctly assigned.

Bonds

Connectivity and bond orders are assigned.

Unbundle

Some external programs output solvent with more than one molecule per residue. This tool operates on active residues recognized or classified as solvent and makes sure they have one molecule per residue.

8. Importing and Exporting Files

Clean Solvent

Acts on active residues recognized or classified as solvent. It adds hydrogens as specified by the Clean Options dialog, adjusts atom types, and corrects bonding.

Molecular Editor For those structures for which QUANTA does not have template information, it is often necessary to go through the process of assigning correct bond orders and/or atom types (one must be correct before the program can determine the other accurately) and adding hydrogens. The Molecular Editor has a complete set of tools designed to do this, particularly aimed at small molecules rather than proteins. This tool in the Split and Clean palette first asks you to select one MSF on which to work and then takes this alone into the Molecular Editor. This is much more efficient than taking in a whole protein–ligand complex.

Structures built within QUANTA by ChemNote or the Molecular Editor itself should not need further editing here.

Auto Edit

Attempts to automatically take a chosen MSF through the Molecular Editor to generate bond orders and atom types and to add hydrogens. Whether this operation is successful critically depends on the initial quality of the structure, i.e., whether it has good enough geometry to determine bond types correctly or if has been typed properly beforehand via dictionaries. An explanatory dialog box is displayed before the edit is attempted. It is up to you to decide whether it would be better to clean up the structure manually.

Clean Nucleics Operates on all active residues classified as nucleic acids. Atom types are assigned using the standard nucleic acid dictionaries, hydrogens are added, retyping is performed as required, and bond orders are determined from these types.

Quit Quits the Split and Clean palette and restores the MSF(s) as they were before entry.

Finish Exits the palette, retaining the new or corrected MSFs.

Exporting an MSF

The **Export** function allows structures in MSFs to be converted to the appropriate format and read into an external database.

Complete the following process to export a file using the PDB format.

1. Select a format.

From the **File** menu, select **Export**, and a File Librarian dialog box opens.

Select 1crn.msf from the scrolling list.

Select the default options:

Atoms to export: All Atoms from MSF

Rotation transformations: Discard

Click the **Export** button.

2. Append remarks to the structure file.

In dialog boxes that offer the opportunity to enter remarks, enter no more than one line of text per dialog box.

Select the **OK** button, and the .pdb file is generated.

9. Using External Applications

This chapter describes the interfaces between QUANTA and a variety of third-party computational chemistry programs. Some of these applications are bundled with core QUANTA; several are additional options. Read this chapter or portions of it to become familiar with access procedures for the following programs:

- Molecular orbital calculations — CINDO and MOPAC
- Poisson–Boltzmann electrostatics and Brownian dynamics — UHBD

As far as possible, the options available within QUANTA cover all functionality in the original versions of these external programs. In addition, the default options in the calculation setup dialog boxes have been specified so that changes are rarely necessary.

Accessing external programs from QUANTA

External third-party programs are automatically started from QUANTA when a request is made for a calculation. While QUANTA requires a graphics workstation for its interactive graphics and molecular displays, the more computationally intensive programs run either on the local workstation or on a range of available network hosts.

Specifying a host

For each third-party application, you may select a host from the list in the `applcomm.db` file, which is customized to contain site-specific information at the time QUANTA is installed.

To select a host for the CINDO, MOPAC, or UHBD applications, display the **Calculate** menu, select **Select Host**, and then select the appropriate application from the pull-right menu.

For all applications, selecting **Select Host** opens a dialog box with a scrolling list of network-available hosts. You can select a different host for each application.

When you select a host, the selection is retained for the duration of the QUANTA session. If no host is specified, QUANTA automatically tries to run the application on your local workstation.

9. Using External Applications

When you select a host, another dialog box opens with fields containing necessary information for running the job over the network. Table 45 lists the options and describes each briefly. Although there already is default information in certain fields, you may change or add more information. This information remains in effect for the entire QUANTA session unless explicitly changed.

Table 45. Select Host dialog box

Data Entry Field	Function
Machine	The name of the host selected from the previous scrolling list dialog box.
Pathname	The full pathname of the program executable on the selected host. Environment variables are valid only if you are running the application on the local machine.
Account	The user ID to run the program on the selected host. A valid user account must exist on the selected host to successfully launch the program.
Password	The password for the user identified in the Account field. A password typed in this field is not revealed on the screen, as all characters are represented as asterisks. By default, no password is used. Depending on site-specific system setup, the host may not require a password to run a remote job.
Working Directory	The directory from which the program is run on the selected host. If the selected host is local, the default working directory is the current QUANTA directory. If the selected host is remote, the default working directory is the login directory of the user identified in the Account field.
Number of Nodes to Use	Number of nodes needed to run the application. Default is 1.

Performing a calculation on a remote host

QUANTA network communication requires one additional program, the remote job remote daemon (RJRD). QUANTA uses RJRD to run each third-party application. After it is started, RJRD establishes a connection back to QUANTA, then receives the path to the third-party application to run and the necessary files to start the program. After the third-party calculation is completed, RJRD sends the resulting file back to QUANTA. RJRD remains active until the calculation is completed and the resulting files are sent back to QUANTA.

Using CINDO

The **CINDO** function in the QUANTA **Calculate** menu provides an interactive interface to the CINDO program (QCPE Program 141). Charges

generated by the program are stored either in a quantum mechanical (QM) coordinate file or incorporated directly into the MSF. Once incorporated into the MSF, these charges can be used in subsequent QUANTA and CHARMM calculations or displayed using the **Label Atoms** function on the **Draw** menu.

The CINDO program has an upper limit of 200 atoms. The options available in the QUANTA interface cover virtually all functionality in the original version of the external programs. The default options in the CINDO calculation setup dialog box have been set up so that changes are rarely necessary. Information on the methods used in the CINDO calculation can be found in Citation 2 in the References section of this chapter.

The CINDO program, although started from QUANTA, can be run in the background so that other QUANTA tasks can be performed during CINDO calculation.

Since CINDO and QUANTA are separate programs, files are used to send information between them. All files associated with a particular calculation have the same user-defined base filename. Table 46 lists the file types associated with CINDO calculations

Table 46. CINDO files

File	Description
filename.cin	Input file to CINDO, automatically created by QUANTA. Contains data that describe the molecular structure and selected calculation options.
filename.out	Log file from the CINDO calculation.
filename.qmc	Quantum mechanical (QM) coordinate file containing the final calculated charges.
CINDO.in	File where CINDO specifically looks for input for running a job.

If you run CINDO in the background, results are not automatically incorporated into the MSF. The calculated atomic charges are stored in the QM coordinate file.

To read the charges stored in the QM coordinate file into the MSF, display the **Calculate** menu and select **Read/Display Results** from the pull-right menu that opens when **CINDO** is selected. A dialog box allows you to choose to:

- Change the current MSF
- Check output for errors
- Report results
- Read charges into the MSF

9. Using External Applications

- Display the dipole moment vector

The contents of the QM coordinate file also can be incorporated into the MSF using the **Import** function in the **File** menu.

All other results to be output can be retrieved from the CINDO.out log file. This file is overwritten when another CINDO calculation is run. To save the data in the log file, change the name of the file at UNIX level.

Complete the following exercise to become familiar with the QUANTA/CINDO interface. To do the exercise, the structure cyclohexanol must be displayed in the QUANTA viewing area. This structure was built in the section *Generating an Electrostatic Potential Energy Surface* in Chapter 6. If you have not completed that section, do so before proceeding.

1. Start CINDO.

Display the **Calculate** menu and select the **CINDO** function. From the pull-right menu that opens, select **Calculate**. A dialog box opens for selecting CINDO options. Table 47 lists these options and provides a brief description of each.

Enter the values:

Title for Calculation: CINDO Calculation on cyclohexanol
Set Charge On System: 0

Select the options:

Specify which Hamiltonian to use: CNDO
Specify Open or Closed Shell Calculation: Closed
Specify Multiplicity: Singlet

Specify the print options:

Minimum - Final energy, partial charges and dipole

Click the **OK** button and a File Librarian dialog box requests the name for a CINDO input file.

Enter the text:

cyclohexanol

Click the **Save** button and the filename extension .cin is automatically added, and a dialog box opens for selecting run options. Table 48 lists the options and provides a brief description of each.

Select the option:

Run in Background

Click the **OK** button and the cursor changes to a watch while the calculation is running. The message line reads:

Submitting CINDO calculation to batch

Other QUANTA functions can be used while the CINDO calculation runs in background mode.

2. Check the status of the CINDO calculation.

Display the **Calculate** menu and select **Show Status**. A dialog box displays a list of background jobs that can be started by QUANTA.

Select the option:

CINDO

Click the **OK** button and the textport reports if the CINDO calculation is in progress or completed.

3. Display the charges for the atoms.

Display the **Draw** menu and select **Label Atoms**. On the pull-right menu that opens, select **Atomic Charge** and the atomic charge assigned by QUANTA is displayed next to each atom.

4. Display CINDO results.

Display the **Calculate** menu and select **CINDO**. From the pull-right menu that opens, select **Read/Display Results** and click the **OK** button. The CINDO Postprocessing Options dialog box opens.

Select the options:

Check output for errors and report results

Read charges into MSF

Display Dipole Moment Vector

Click **tns**, select **Atomic Charge** and the atomic charge is assigned by the **OK** button.

A File Librarian dialog box requests the name of a CINDO output file. The filename extension .out is automatically contained in the data entry field.

Select the entry:

cyclohexanol.out

Click the **Open** button and the calculation results are displayed in the textport. In a dialog box that offers the option of saving the structure, select the option:

Create New Generation of cyclohexane.msf

Click the **OK** button. The dialog box is cleared from the screen, the textport indicates that the old structure file is renamed cyclohexanol.msf,002, and the new charges are saved in cyclohexanol.msf. The atom labels are also changed to reflect the new CINDO-generated charges.

The dipole moment vector, a graphical object, is displayed in the viewing area. The Object Management Table opens, listing Dipole_1.

5. Delete the dipole moment vector.

Select the **Delete** cell for Dipole_1. The text changes from **no** to **yes**, the dipole moment vector is no longer displayed, and the Object Management Table closes.

6. Delete the labels for the structure cyclohexanol.ene.

Display the **Draw** menu and select **Label Atoms**. From the pull-right menu that opens, select **Off** and the labels are no longer displayed.

Table 47. CINDO Setup options

Option	Description
Title for Calculation	Offers a data entry field to enter an optional title. If a title is entered, it appears at the top of the input file and log file.
Set Charge on System	Allows the charge on the system to be specified. The value contained in this field is the nearest integer to the current net charge of the structure.
Specify which Hamiltonian to Use	Opens a dialog box for selecting which Hamiltonian options to use in the calculation. The CNDO Hamiltonian (CNDO/2) is the default.
Specify Open or Closed Shell	Opens a dialog box for selecting an open- or closed-shell calculation to analyze the molecule. The default is Closed Shell Calculation .
Specify Multiplicity	Opens a dialog box for selecting the structure multiplicity (singlet, doublet, or triplet). The default is singlet multiplicity.
Specify Print Options	Opens a dialog box selecting the amount of output generated in the CINDO log file, CINDO.out. This log file is overwritten by later CINDO runs. To save the data it contains, the name of the log file must be changed at the UNIX level.

Table 48. CINDO Run options

Option	Description
Run Calculation Now	Runs CINDO in foreground mode, which halts other QUANTA tasks. A QM coordinate file, <i>filename.qmc</i> , is created to store the results of the completed calculation.
Run in Background	Runs the CINDO calculation in the background and stores the charges in the QM coordinate file, <i>filename.qmc</i> . Other tasks in QUANTA can be performed while CINDO is running.
Do Not Run Save Input File(s)	Stores the specifications for the calculation in an input file, <i>filename.cin</i> . This file can be reloaded to run a CINDO calculation later.

Using MOPAC

MOPAC is a semi-empirical molecular orbital program that is generally used in the study of chemical reactions and molecular structure problems. The interactive interface allows you to run the MOPAC program and display some of the results within QUANTA. For example, you can process results of calculations to obtain molecular orbitals and display them as graphical objects.

Versions of MOPAC that can be used with QUANTA include MOPAC 5 and MOPAC 6. MOPAC 93 is not known to work.

The semi-empirical Hamiltonians available within MOPAC include:

- PM3
- AM1
- MNDO
- MINDO/3

Available calculations include:

- Vibrational frequencies
- Thermodynamic quantities
- Polarizability
- Isotopic substitution effects
- Geometries

In MOPAC, calculations may be performed when more than one molecular structure is selected, for example, during drug docking studies. However, do not perform MOPAC calculations on multiple molecules that are not

9. Using External Applications

connected by covalent bonds. If MOPAC results are to be read back into QUANTA, all selected structures must be contained in a single MSF.

MOPAC creates a series of files for each calculation. All files associated with a particular calculation have the same user-defined base filename.

Table 49 lists the files and provides a brief description of each.

Table 49. MOPAC files

File	Description
filename.ain	Input file to MOPAC.
filename.out	Log file from the MOPAC calculation.
filename.arc	Archive file containing a short summary of the calculation results (final heat of formation, dipole moment, geometry, etc.).
filename.shu	Shutdown file automatically created by the Shutdown MOPAC option. Writing anything to this file shuts down MOPAC, creating <i>filename.den</i> and <i>filename.res</i> for restarting the calculation.
filename.den	Density matrix file automatically created during normal shutdown. This file is needed for the Restart Calculation option.
filename.res	Restart file automatically created during normal shutdown. This file is needed for the Restart Calculation option.
filename.gra	Results file containing calculation results in a form suitable for processing into graphical output (for example, orbital and electron density maps).
filename.qmc	Quantum mechanical (QM) coordinate file containing the final Cartesian coordinates and calculated charges.
filename.qpt	Results file containing the dipole moment vector for the calculated structure

Complete the following exercises to learn the basics of using the QUANTA MOPAC application. The exercises use *cyclohexanol.msf*, which was built in the *Electrostatic Potential* section of Chapter 6. If you did not complete that section, do so before proceeding.

1. Display a structure.

From the **File** menu, select **Open**. From the scrolling list in the Open MSF File Librarian, select *cyclohexanol.msf*.

Select the option:

Replace

Click the **Open** button and the structure cyclohexanol is displayed in the viewing area.

2. Start the QUANTA/MOPAC interface.

Display the **Calculate** menu and select the **MOPAC** function. From the pull-right menu that opens, select **Calculate**.

3. Run a MOPAC/AM1 calculation.

Select the option:

Set up Calculation

Select the **OK** button and the Setup MOPAC Calculation dialog box opens.

Fill in (or leave the default) for the title for the calculation:

MOPAC calculation on cyclohexanol

Select the options:

AM1

Z-matrix with Automatic Setup

Enter the value:

Molecular charge: 0

Click the **OK** button and the Geometry Optimization Options dialog box opens.

Select the option:

Full Geometry Optimization

In the File Librarian dialog box that opens, enter the text:

cyclohexanol

Click the **Save** button and the input file cyclohexanol.ain is saved. In the MOPAC Run Options dialog box that opens, select the option:

Run Calculation Now

Click the **OK** button. This sends the coordinates and element types to MOPAC and starts the MOPAC calculation. This calculation takes several minutes since a geometry optimization (energy minimization) is requested. For large molecules, run calculations of this type in the background. The textport reports the progress of the MOPAC calculation.

4. Process MOPAC results and incorporate them into the MSF.

After the calculation finishes, the MOPAC Postprocessing Options dialog box opens.

Select the options:

9. Using External Applications

Check output for errors and report results

Read coordinates into MSF

Read charges into MSF

Select the **OK** button. In the MSF Saving Options dialog box, select the option:

Save to New Filename

In a File Librarian dialog box that opens, enter a new filename:

cyclohexanol_mo

Select the **Save** button to save the MOPAC-generated structure. This ensures that the molecule on the screen has the same Cartesian coordinates as the molecule saved in the MSF file. It permits comparison between the initial cyclohexanol structure (cyclohexanol.msf) and the MOPAC-processed cyclohexanol structure (cyclohexanol_mo.msf). QUANTA automatically returns to Molecular Modeling mode.

5. Display MOPAC AM1 results – Bond lengths.

Display the **Calculate** menu and select **Internal Coordinates**. From the pull-right menu that opens, select **Bond Lengths** and the Select Atoms and Selection Utilities palettes open.

From the Select Atoms palette, select **Include** and **All Atoms**.

Select **Finish**. The palettes close and a dialog box asks for directions about what to report when both atoms in a bond are selected.

Select the option:

Report bond length once only

Select the **OK** button and a list is displayed in the textport showing the bond assignments and lengths. The atom labels for defining the bonds are the same as those shown on the structure in the viewing area.

This same procedure can be used to display a list of bond angles or dihedral angles. The only difference is in the selection from the **Internal Coordinates** pull-right menu.

6. Display bond lengths in the viewing area.

From the Geometry palette, select **Distance** and **Show Distance Monitors**.

Pick any two carbon atoms. The bond length between them is displayed in the viewing area in the space between the two atoms picked. The bond length is the same as that listed earlier in the textport.

Continue picking atom pairs to display other bond lengths. Use **Delete Distance Monitors** in the Geometry palette to remove reported bond lengths from the screen. Deselect **Distance**.

Executing a single-energy AM1 calculation

AM1 (Austin Model 1) is parameterized to be especially useful for hydrocarbons and other polar structures that have appreciable hydrogen bonding interactions. For more information about this calculation, see citation 3 in the references section of this chapter.

1. Set Up the AM1 Calculation.

Display the **Calculate** menu and select **MOPAC**. In the Select MOPAC option dialog box, select the option:

Setup Calculation

Click the **OK** button. In the Setup MOPAC Calculation dialog box, select the option:

AM1

Click the **OK** button. In the Geometry Optimization Options dialog box, select the option:

No Geometry Optimization

Click the **OK** button. In the File Librarian dialog box, enter the text:

cyclohexanol_single.ain

Select the **Save** button and the MOPAC Run Options dialog box opens.

2. Run MOPAC.

Select the option:

Run Calculations Now

Select the **OK** button and the MOPAC calculation starts.

3. Display the results.

When the calculation is complete, the MOPAC Post Processor Options dialog box opens.

Select *only* the option:

9. Using External Applications

Create MO or Charge Density Map

Select the **OK** button. In the Molecular Orbital Postprocessing dialog box, enter the values:

Select the MO [HOMO]: 21

Grid points per map edge: 20

Conformation Number: 1

Select the options:

Molecular Orbital Map

Wait for Calculation to Complete

Click the **OK** button.

The orbitals are calculated for the coordinates of the molecule as it appears in the viewing area. When you run this calculation, the molecule should not be moved relative to the saved MSF.

When the calculation of the orbitals is completed, a default name for the graphical object, MOLORB1, is offered.

Click the **OK** button to accept the name, and the Object Management table is displayed with MOLORB1 listed.

In a dialog box that lists display options for the brick map, select the option:

All of the map displayed

Select the **OK** button and the dialog boxes for displaying the objects open. In each of the dialog boxes, accept the defaults for contour levels as well as the colors associated with them.

The brick map is displayed on the screen.

4. Delete the brick map object.

Select the **Delete** cell in the Object Management Table for MOLORB1. The text changes from **no** to **yes**, the brick map is removed from the screen, and the Object Management Table closes.

5. Repeat the calculation using a different Hamiltonian.

To obtain data to compare with AM1, rerun the MOPAC calculation, Steps 1 through 4, using the Hamiltonian PM3 instead of AM1.

Table 50. MOPAC pull-right menu

Selection	Description
Calculate	Establishes specifications for the calculation.
Use Input File	Starts a calculation with a previously created input file.
Read/Display Results	Reads results of calculations and creates an MSF containing the results.
Restart MOPAC	Restarts a shut down MOPAC calculation.
Shutdown MOPAC	Stops a MOPAC calculation in progress.
Cleanup Files for MOPAC	Calls a File Librarian for choosing data files to be cleaned up (deleted).

Table 51. Set Up MOPAC Calculation dialog box

Option	Description
Title for Calculation	Title for the calculation to be performed.
Specify Which Hamiltonian To Use	
PM3	Performs calculation using PM3 Hamiltonian.
AM1	Performs calculation using AM1 Hamiltonian.
MINDO	Performs calculation using MINDO Hamiltonian.
MINDO/3	Performs calculation using MINDO/3 Hamiltonian.
Specify Input Format	
Z-Matrix with Automatic Setup	Automatically creates a z-matrix (internal coordinate table) to specify the initial geometry. The starting chain includes nonhydrogen atoms and excludes terminating groups such as methyl.
Z-Matrix with User Specified Order	Specifies the atom ordering of the z-matrix.
Cartesian Coordinates	Indicates that the input file contains Cartesian coordinates (not z-matrix). Useful for comparing similar systems. Geometry optimization is limited to all or nothing. Symmetry constraints cannot be applied.
Setup Dummy Atoms in the Z-Matrix	Allows dummy atoms to be created and included in the z-matrix. Allows the formation of dummy bonds linking fragments. Essential for reaction coordinate studies.
Use Symmetry Constraints	Simplifies optimization by requiring bond lengths, angles, and torsion angles to equal those for reference bonds, angles, and torsions.
Molecular Charge	Specifies the net charge on the structure.
Other Options	Displays a dialog box of several advanced options.

Table 52. MOPAC Geometry Optimization options

Option	Description
Full geometry optimization	Optimizes all bonds, angles, and torsion angles.
All bonds only	Optimizes only bond lengths.
All angles only	Optimizes only the bond angles.
All torsion angles only	Optimizes only the torsion angles.
User selected parameters	Opens a palette with selections to control which bond lengths, bond angles, and torsion angles are optimized.
No geometry optimization	Performs no geometry optimization.

Table 53. MOPAC Post Processing options

Option	Description
Check Output for errors and report results	Checks the .out and .arc files for error messages. Also reports some results. If the MOPAC run fails, some post-processing options are invalid and corresponding results files are not created. If this option detects a fatal error, selected post-process options are not performed. If warning messages are encountered, you are given the choice of continuing or not. Use of this option is strongly recommended.
Make .qmc and dipole file for different conformation	Allows data to be processed to form individual files containing coordinates and charges that can be read into QUANTA MSFs and .qpt files for the corresponding dipole vectors.
Read Coordinates into MSF	Extracts coordinates from the .qmc file and updates the MSF with them.
Read Charges into MSF	Extract the charges from the .qmc file and updates the MSF with them.
Create .csr File	Stores conformers in a .csr file that can be studied later using the Analysis application.
Display Dipole Moment Vector	Retains the dipole moment information in the form of a QUANTA plot file (.qpt), so that the vector can be displayed as a graphical object.
Create MO or Charge Density Map	Processes molecular orbital data for a QUANTA .mbk file containing a contoured map of specified molecular orbitals or the corresponding charge density. If a reaction coordinate study was performed, maps can be generated for the different structures.
Cleanup Files	Presents a list of files created for the MOPAC run and allows their selective deletion. The files are ordered so that the files least likely to be needed again are at the top of the list.

Comparing MOPAC data

MOPAC AM1 and PM3 data for cyclohexanol, along with similar data from calculations using CHARMM, are reported in Tables 54, 55, and 56. How atom numbers were assigned in these tables depends on how the structure was built, so there may not be a ligand with the data you generate.

Table 54. Comparison of bonds

Bond	CHARMM	AM1	PM3
H-O	0.950	0.964	0.949
O-C1	1.411	1.418	1.409
C1-C2	1.538	1.527	1.537
C2-C3	1.534	1.513	1.520
C3-C4	1.535	1.516	1.520

Table 55. Comparison of angles

Bond	CHARMM	AM1	PM3
H-O-C1	109.7	107.3	107.4
O-C1-C2	111.9	111.0	112.0
C1-C2-C3	110.7	110.6	110.6
C2-C3-C4	111.1	111.3	111.1
C2-C1-C6	111.1	110.9	110.4

Table 56. Comparison of ring torsions

Torsion	CHARMM	AMI	PM3
C1-C2-C3-C4	56.3	56.1	56.8
C2-C3-C4-C5	56.0	56.0	56.4
C3-C4-C5-C6	55.9	56.0	56.1

Using UHBD

The QUANTA/UHBD interface simplifies the process of creating input for and running the University of Houston Brownian dynamics (UHBD) program. The interface provides access to these UHBD applications such as:

- Electrostatic calculations for macromolecules in solution using the Poisson–Boltzmann equation
- Calculation of diffusion-controlled rate constants using Brownian dynamics

The QUANTA/UHBD interface provides tools for displaying results of UHBD calculations. A 3D contour mesh of the electrostatic potential, the electrostatic potential, and Brownian dynamics trajectories may also be displayed superimposed on the structure. Manipulation of these types of graphic objects is discussed in Chapter 6.

Summary

QUANTA provides access to several external programs that provide alternative or supplemental approaches to modeling. These include:

- Molecular orbital calculations — CINDO and MOPAC
- Poisson–Boltzmann electrostatics and Brownian dynamics — UHBD

As much as possible, the options available within QUANTA cover all functionality within the original versions of these programs. In addition, the default options in the calculation setup dialog boxes have been specified so that changes are rarely necessary.

External third-party programs are automatically started from QUANTA when a request is made for a calculation. While QUANTA requires a graphics workstation for its interactive graphics and molecular displays, these computationally intensive programs may be run either on the local workstation or on a range of available network hosts.

Following is a brief summary of each program documented in this chapter.

CINDO

The CINDO program (QCPE Program 141) is a molecular orbital program supplied by the Quantum Chemistry Program Exchange, Department of Chemistry, Indiana University. The program has an upper limit of 200

atoms. Options available within the QUANTA interface cover virtually all functionality within the original version of the external programs.

Charges generated by the program are stored in a quantum mechanical (QM) coordinate file or incorporated directly into the MSF. Once incorporated into the MSF, these charges can be used in subsequent QUANTA and CHARMM calculations or displayed.

MOPAC

MOPAC (QCPE 445) is a semi-empirical molecular orbital program that is generally used in the study of chemical reactions and molecular structure problems. It is also provided by the Quantum Chemistry Program Exchange, Department of Chemistry, Indiana University.

The semi-empirical Hamiltonians available within MOPAC include:

- PM3
- AM1
- MNDO
- MINDO/3

Available calculations include:

- Vibrational frequencies
- Thermodynamic quantities
- Polarizability
- Isotopic substitution effects
- Geometries

UHBD

The QUANTA/UHBD interface simplifies the process of creating input for and running the University of Houston Brownian dynamics (UHBD) program and provides tools for displaying results of UHBD calculations. The interface provides access to UHBD applications:

- Electrostatic calculations for macromolecules in solution using the Poisson–Boltzmann equation
- Calculation of diffusion-controlled rate constants using Brownian dynamics

References

- Information on CINDO and MOPAC can be obtained from QCPE documentation obtained from the Quantum Chemistry Program Exchange, Department of Chemistry, Indiana University.
- See CINDO calculation methods in *Approximate Molecule Orbital Theory*, J. A. Pople and D. L. Beveridge, McGraw Hill Inc., New York, 1970.
- See MOPAC AM1 calculation methods in *Reviews in Computational Chemistry*, Chapter 2, K. S. Lipkowitz and D. B. Boyd, VCH Publishers, New York, 1990.

Index

\$CHM_DATA directory 67
\$HYD_LIB/symlib.sym 98
2D molecule 5
 assign charges 33
 change atoms 15–18
 create 11–??
 customize bonds 19–20
 save 20–23
2D sketch 11
2dpartial.epo 142
3D Builder, see Molecular Editor 41
3D Molecular Editor Save Options dialog box 59
3D structure
 alter 47
 create 39–41

A

Add Atoms palette 47
 Convert to Hydroxyl 50
.ain file 194
AMINO.RTF 85, 92
Applications menu
 Builders 6, 40, 41
 Crystal Modeling 97–106
 Protein Design 107
 Protein Health 107
 Protein Profile Analysis 107
.arc file 194
artist plot
 user-defined commands 174
.asd file 98
asymmetric unit 98
 modify 102–??
atom
 alter 47–52
 retype 49
Atom Table 60
Atom Table headings 61

B

bond icons 12–14
bond stretching 77
brick map 122, 126
 delete 129, 130
 display 123, 128
 reconstruct 129
Builders menu
 2D Sketcher 6, 40
 3D Builder 41
 Sequence Builder 79, 82

C

Calculate Electrostatic Field palette
 Calculate 2D Slice 143
 Calculate from Partial Charges, 143
 Define Plane 143
 Display Results 144
Calculate Electrostatic Potential palette 138, 139
 Calculate 2-D slice 141
 Display Results 138, 140
Calculate menu
 CINDO 188–192
 Electrostatics 134–144
 Hydrogen Bond 144, 148
 Interaction Maps 123, 127
 Internal Coordinates 196
 MOPAC 193–??
 Solvent Surfaces 117–122
 UHBD 202–??
carbon substitution 15
Cartesian coordinates 67
Categories Table 45
CCK7 91
CCK7.msf 93
CHARMm calculations 67
CHARMm data sources 66

- CHARMm energy functions 65
 - CHARMm menu 68
 - CHARMm mode 77
 - Get Fourth Parameter 114
 - Minimization Options 52, 72, 73
 - Update Parameters 101
 - CHARMm minimization, see minimization
 - CHARMm operations 65–69
 - CHARMm parameter file 66
 - charmm.img 102
 - charmm_img.str 102
 - CHARMm-QUANTA interaction 67
 - ChemNote 39
 - start 5
 - ChemNote Edit menu
 - paste 27
 - ChemNote File menu 7
 - Save 21
 - Template 28
 - ChemNote Information menu 7
 - ChemNote Layout menu 30
 - ChemNote menu bar 6
 - ChemNote Message Line 11
 - ChemNote palette 10, 30
 - Cis/Trans 22
 - ChemNote Properties menu
 - Atom Properties 33
 - ChemNote template 26–36
 - ChemNote window 6
 - .cin file 189
 - CINDO
 - calculate 190–192
 - files 189
 - run options 193
 - setup options 190, 192
 - CINDO menu
 - Read/Display Results 189
 - CINDO, also see Calculate menu 188
 - CINDO.in 189
 - CINDO.outlog file 190
 - cis.mol 23
 - cis.msf 25
 - Color Atoms palette 165
 - color scale 116
 - Color Schemes and Utilities palette 165
 - complex_dna.msf 163
 - Connolly solvent surface, see Calculate menu 117
 - contour level 124, 128
 - contour map 126
 - Create Objects 114
 - crystal
 - calculate energy 99–102
 - enter dimensions 105
 - Crystal Modeling
 - real atom mode 98
 - see Applications menu 97
 - symmetry atom mode 98
 - Crystal Modeling palette 99
 - CHARMm Energy/Image 101
 - Minimize Crystal 106
 - Modify Asymmetric Unit 102
 - Modify Symmetry Copies 106
 - .csr file 181
 - cyclic peptide
 - apply patches 92
 - create 91–94
 - minimize 93
 - cyclohexanol 135
 - cyclohexanol.ene 192
 - cyclohexanol.msf 192, 194
-
- D**
- .den file 194
 - Dial Emulator 46
 - Dial Set 2 Fragment & Set Transformation Dials 58
 - Display Field palette 144
 - Display Potentials palette 140
 - Set Contour Levels 138
 - Show 1-Molecule Potential 138
 - Draw menu
 - Color Atoms 165
 - Create Objects 113, 114, 115, 124
 - Object Parameters 112
 - Raster Models 169
-
- E**
- Edit Atoms palette 48
 - Type All Atoms 49

- Edit Bonds palette 44
 - Display Kekule Structures 44
- Edit menu
 - Atom Data 39, 62
 - Atom Property Editor 39, 60
 - Bond Options 39, 62, 145
 - Incorporate Data 114
 - Molecular Editor 39, 43
- Editor Options dialog box 53
- electrostatic field
 - calculate 143–144
- electrostatic interactions 77
- Electrostatic menu
 - Field 143
 - Potential 138
- electrostatic potential
 - 2D isoenergetic contour plot mode 134
 - 3D surface mode 134
 - calculate 134–142
 - calculate isoenergy 2D contour plot 141–142
 - calculate using VSS method 134
 - display dot surface 139
 - display grid map 135–139
- external programs
 - access from QUANTA 187–188

F

- fieldcalc program 143
- file format
 - Import/Export 179
- File menu
 - Export 179, 185
 - Import 179, 181
 - Plots 169
 - Save As 39
- Fourth Parameter menu
 - Forces 114
- Fragment Table 45
 - Functional Groups 45
 - Toggle Icons 45

G

- Geometric Structure Definition files (gsd) 183

- Geometry palette
 - Distance 70
 - Show Distance Monitors 70
- Get Fourth Parameter 114
- .gra file 194
- graphical object 155
 - display 111
 - display during movement 159
 - generate 111
 - manage ??–117
- grid contour mesh
 - define grid 113
 - generate 113–114
 - generate from selected atoms 114
- grid intersection 124

H

- hard copy plot options 170
- Host
 - remote calculation 188
- hydrogen
 - manipulate 17, 49
- hydrogen bond
 - apply to other structures 150
 - default parameters 145
 - generate 144–151
- hydrogen bond acceptor 145
- hydrogen bond donor 145
- Hydrogen Bonds palette 151
 - Calculate Hbonds 148
 - Set Parameters 148

I

- image 99
- Import 181
- Incorporate Data 114
- Incorporate Data menu
 - Vectors 114
- Interaction Maps menu
 - Molecule 127
 - Probe 123
- Internal Coordinates menu
 - Bond Lengths 196

M

- .mbk file 122
- Merck Molecular Force Field 76
- methanol.mol 56
- methanol.msf 57
- minimization 71–76
 - repeat 74
 - save results 75
- Minimization Options dialog box 72
- minimization techniques 72
- MMFF energy expression 77
- Model Asymmetric Unit palette 102
- Modeling palette
 - CHARMm Energy 52, 71
 - CHARMm Minimization 73, 74
 - Hydrogen Bond 145, 150
 - Move Atom 70
 - Move Fragment 25
 - Reject Changes 75
 - Save Changes 26, 70, 75
- .mol file 5, 21
- mol_inter.mbk 130
- Molecular Editor 182
- Molecular Editor palette 41
 - Add All Hydrogens 49, 52
 - Add Atoms 47
 - Add Polar Hydrogens 49
 - Change Atoms 47
 - Change Bond 43
 - CHARMm Minimize 52
 - Delete Atoms 51
 - Delete Hydrogens 49
 - Display Atom Labels 48, 50, 51
 - Display Fragment Table 45
 - Edit Atoms 48
 - Edit Bonds 44
 - Editor Options 48, 54
 - Merge Fragment 46
 - Move Fragment 46, 58
 - Save and Exit 55, 59
- Molecular Modeling
 - import 24–26
 - return from ChemNote 23–24

- Molecular Probe Interaction Options dialog box 132

- molecule interaction 125–132

- Molecule Management Table 57

- Molecule window 155

- MolScript interface 174

MOPAC

- AM1 calculation 197–198

- calculations 193

- compare data 201

- geometry optimization options 200

- Hamiltonians 193

- post processing options 200

- MOPAC files 194

- MOPAC menu 199

- MOPAC Postprocessing Options dialog box 195

- MOPAC versions 193

- MOPAC, see Calculate menu 193

MSF

- calculating solid surfaces from 166

- export 184

- .msf file 181

- mypeptide 89, 160

- mypeptide.msf 91, 112, 147

N

- newpeptide.msf 6, 151

- nitrobenzene.msf 104, 118, 122

- NMR Structure Determination 108

- nucleic acid cartoon 163

- set up parameters 164

O

- Object Creation dialog box 112, 113

- Object Management 166

- Object Management Table 111, 113, 116, 124, 129, 155, 161

- Object Parameters menu

- Ribbon Parameters 112

- orange.msf 34, 65, 70

- orthogonalization code 99

- .out file 189, 194

- out-of-plane bending at tri-coordinate centers 77

P

patch residue 84
 .pct file 5
 PDB file renaming 180
 PDB, see Protein Data Bank
 peptide
 create 87–90
 minimize 90–91
 secondary conformation 87
 phenol.mol 40
 phenol.msf 41
 plot
 disposition options 171
 preview 171
 Plot Molecules menu
 Generate 172
 potential energy
 generate a value 70–71
 Preferences menu
 PDB Import/Export 180, 181
 probe 122
 probe interaction 122–124
 probe interaction energy 122
 Probe Interaction Options dialog box 125
 Prompt for Multi-Model options 181
 Property Editor palette 60
 Atom Table 60
 protein cartoon 163
 set up parameters 163
 Protein Data Bank data format 181
 Protein Data Bank files
 importing 181
 Protein Design 107
 Protein Health 107
 Protein Profile Analysis 107
 protein_structre.gsd 183
 PSF 5, 66

Q

.qmc file 189, 194
 .qpt file 115
 .qpt file 194

R

raster model 169
 Raster Models menu 169
 raytrace model 168
 Remote Job Remote Daemon 188
 rendering styles 155
 .res file 194
 residue 84
 Residue Table 60, 62
 Residue Table headings 62
 RGB graphics 155
 ribbon
 generate 112–113
 ring icons 11
 RJRD 188
 RTF 5, 66, 83

S

Save Changes Options dialog box 69
 search1.msf 57, 126
 Select Atoms palette 118, 196
 Select Host Dialog Box 188
 Selection Utilities palette 118, 196
 .seq file 87
 .STR file 87
 sequence
 build 84–??
 Sequence Builder
 see Builders menu 79
 start 82
 Sequence Builder Conformation menu 84
 Set Secondary Conformation 88, 92
 Sequence Builder Data menu 82
 Delete Sequence and Restart 86
 Sequence Builder Edit menu 83
 Apply Patches to Residues 92
 Copy Marked Item 85
 Delete Marked Item 86
 Scroll Down 86
 Scroll Up 86
 Unmark Items 86

Sequence Builder menu 81
Sequence Builder Message Line 81
Sequence Builder palette 81
Sequence Builder window 80–81
Set Up MOPAC Calculation dialog box 199
.shu file 194
sodium.msf 34, 65, 70
Solid Display palette 156, 162
 Protein Backbone 162
solid model
 create ??–163
 generate cartoon 163–??
 hardware requirements 155
 manipulate 157–??, 157–159
Solid Model Settings 161
Solid Model window 155, 159–??
 popup menu 159
 settings selections 160
 stereo selections 160
Solid Models menu 155
 Ball and Stick 161
 Liquorice 161
Solid Schemes and Utilities palette 156, 158, 162
Solid Surfaces 166
solvent surface map
 recreate 119
Solvent Surface Options dialog box 118, 120
solvent surface, see Calculate menu 117
space group 105
Split and Clean 182
 Cleaning Tools 183
 Splitting Tools 182
stretch-bend interactions 77
structure
 adjust charge 60
 combine 56
 minimize 52–53
 rename 76
 rotate 47
 save 53–60
 save multiples 56
 selection options 23
Surface Display Options dialog box 119, 121
symmetry copies 98
symmetry library file 98

T

Table 38 159
Template Viewer window, see Template window
Template window 27
 menu bar 27
 title bar 27
Template window button 27
Template window menus 27
template, also see ChemNote template
torsion interactions 77
trans.mol 22
trans.msf 25

U

UHBD, also see Calculate menu 202
unit cell dimensions 99
unit cell parameters 98

V

van der Waals interactions 77
vector data
 transferring 114
vectors 114

W

water probe 126
water.msf 128

X

X-Ray 108