VSEPRplex DEMO HELP CONTENTS

COMPUTER SCIENCE

ABOUT VSEPRplex

VSEPRplex (pronounced "ves-per-plex") is a molecular modelling set, which uses the computer to assist studies in VSEPR theory. The title, "VSEPRplex," is a "portmanteau word" in that it blends the sounds and combines the meanings of two words, "VSEPR" and "perplex." This joining suggests the purpose of the program: to help students overcome the visual and conceptual perplexities that are so often a part of studying VSEPR theory.

The main reason why many students have difficulty with VSEPR theory is that the traditional teaching aids have never been very effective. The concept of three-dimensional bonding is not easily conveyed, and blackboard illustrations and physical modelling sets do not meet the challenge well. Drawings are particularly poor because it is most difficult to accurately reproduce proportion and perspective in two-dimensions. As well, the fact that drawings are static (i.e., students see only one "view" of a molecule) makes them even less desirable. Physical modelling sets are something of an improvement, but even these can be frustrating. Modelling sets limit the number of molecules that can be assembled, and forfeit or compromise important attributes, such as atomic radii, bond angles and bond distances.

VSEPRplex overcomes these kinds of problems in two ways. To begin with, the program frees molecular modelling of all physical restraints by creating simulations that exist only in the computer. This "virtual" process provides models that are exceptionally flexible, detailed and accurate. A second advantage is that molecules are "generated" in the true sense of the word. VSEPRplex does not simply retrieve its models from a molecular database; for any particular molecule, the program mathematically derives the structure from first principles of physics and chemistry. This guarantees that almost any molecule predicted by VSEPR theory can be modelled with VSEPRplex. As well, by generating molecules, the program provides clear evidence as to the utility of the theory.

Modelling with VSEPRplex is powerful, but the process is easily mastered. The student assembles a formula by using the mouse to select elements from a periodic table. The program then models the structure. Four models of the molecule (skeletal, Lewis, wire-frame and space-filling) are available. These models have unique qualities, and together they provide the student with a solid representation of the molecule. Perception can be further enhanced by performing "real-time" rotations on the three-dimensional models, and by adjusting various features of the models (e.g., the choice of rendering, shape classification, etc.). As well, models are accompanied by text displays, which tutor the student in structural derivation procedures. All in all, VSEPRplex provides the student with the opportunity to realize both visual and conceptual proficiency with VSEPR theory. The aim is to make molecular bonding something that the student truly understands.

ABOUT THE AUTHORS

Christian and Shawn are originally from Espanola, a small pulp and paper town in Northern Ontario. Peter is from Kingston, Ontario, the city where all three met and are currently attending university. The authors have long been programming enthusiasts, and they continue to devote much of their spare time to the design of new and innovative software.

"VSEPRplex", their most involved effort thus far, was initiated in 1990 by Christian and Shawn. While developing the program, they were twice chosen to represent Espanola and the North Channel region at the annual Canada-Wide Science Fair (CWSF) competition. At CWSF '90, held in Windsor, Ontario, they were awarded the silver medal for Senior-level Computer Science. After further developing the program, Shawn travelled to Vancouver, British Columbia for CWSF '91, and there received the national gold. Peter joined the team in 1993 to develop a Windows version of the program, and has made invaluable contributions to the project design as a whole. VSEPRplex is currently available for Microsoft Windows and Apple Mac OS (68K and PPC).

In addition to software design and chemistry, Christian enjoys writing, drawing and playing the classical guitar. In 1993, he received a philosophy degree from Laurentian University in Sudbury, Ontario. He is currently attending Law School at Queen's University.

Shawn's many hobbies include taking part in local theatrical productions, playing the bass-guitar and exploring the numerous applications of fractal geometry and Chaos theory. He is currently enrolled in a mathematics programme at Queen's University.

Peter enjoys making wine, participating in student organizations and playing the classical guitar. He is presently studying mathematics at Queen's University, and hopes to enter graduate studies upon completing his degree.

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Thank you for supporting a student project.

VSEPRplex DEMO

With this demo of VSEPRplex (pronounced "ves-per-plex") only the water molecule (H_2O) can be modelled. The complete package will have to be purchased before the many other molecules predicted by VSEPR theory can be explored. See the Fundamental Structures reference chart for a list of just some of the molecules predicted by this theory.

VSEPRplex PRICE LIST
JULY 1995

VSEPRplex is available for **Microsoft Windows** and **Apple Mac OS (68K and PPC)**.

STUDENTS AND OTHER PERSONS

PRICE = $30 CDN / $24 U.S. for each package.

HIGH SCHOOLS, COLLEGES, UNIVERSITIES, ETC.

PRICE = $100 CDN / $80 U.S. for initial package + $20 CDN / $16 U.S. per additional copy.

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SYSTEM REQUIREMENTS

In order to use the VSEPRplex Demo, the following equipment is required: a computer running Mac OS Version 7.0 (or later) with 640K of free memory, a mouse and a colour monitor.

For installation instructions, see Installation.

INSTALLATION

Before installing the VSEPRplex Demo, make a back-up of the VSEPRplex Demo disk, and then store the original disk in a safe place.

The VSEPRplex Demo can be run from a floppy disk, but will operate faster from a hard drive. To install the VSEPRplex Demo on a hard drive, simply drag the **VSEPRplex Demo folder** to the desired location on the hard drive.

For loading instructions, see Loading. For information on system requirements, see System Requirements.

LOADING

To run the VSEPRplex Demo, open the **VSEPRplex Demo folder**, and then double-click on the **VSEPRplex Demo application icon**.

For installation instructions, see Installation.

TUTORIAL

This tutorial gives an overview of the molecular modelling process with VSEPRplex. A more detailed explanation of the program's functioning can be found in the **Reference section**.

The molecule to be modelled is water (H_2O), a substance familiar to everyone. Before the modelling process can begin, the molecule's formula has to be entered. This is achieved by selecting elements in their appropriate quantities from the periodic table of the elements. The periodic table is found in the **Formula window**. Each element on the periodic table is a "button," which can be selected with the mouse. Click twice on the **Hydrogen button** with the mouse button. Note: If the mouse has more than one button, use the left mouse button. This inserts two atoms of hydrogen into the formula. Click once on the **Oxygen button** with the mouse button. This inserts one atom of oxygen. The formula now reads "H_2O" in the **Formula window**.

A delete function is available for making corrections to the formula. Insert a second oxygen atom into the formula. The formula now reads "H_2O_2." Hold down the **Shift key**, and click once on the **Oxygen button** with the mouse button. This removes the second atom of oxygen from the formula.

It is possible to ionize (i.e., place a charge on) the molecule. To the right of the periodic table are two **Ion buttons**. Click on the **Positive Ion button** three times. This gives the formula a charge of +3. Click on the **Negative Ion button** three times. This makes the water molecule neutral again, as it should be.

At this point, it is useful to view attribute data for the elements in the formula. Use the mouse to pull down the **Text menu**, and select the **Element Attributes item**. This displays the element attributes (e.g., atomic number, covalent radius, etc.) for hydrogen and oxygen in the **Text window**. These values are used by VSEPRplex when it calculates the structure of the molecule. The attribute data is made available to encourage users to perform the structural calculations by hand.

The actual modelling now begins. To the lower right of the periodic table is a **Model button**. Click on the **Model button**. This instructs VSEPRplex to analyse the formula to determine whether it satisfies VSEPR theory. If the elements, in their given quantities, are incompatible, a window opens and communicates the problem and a solution. Since H_2O is a valid combination of elements, the program accepts the formula, and displays structural calculations (which outline how the shape of the molecule was determined) in the **Text window**. As well, a two-dimensional skeletal model is displayed in the **Model window**. This is the simplest model.

Four different models of the molecule are available: skeletal, Lewis, wire-frame and space-filling. Pull down the **Model menu** and select the **Lewis item**. The skeletal model is replaced with a more informative Lewis model. The Lewis model is also two-dimensional, but unlike the skeletal model, it reveals lone pairs, as well as the allocation and types of bonds in the

molecule. Notice how these details relate to the structural calculations in the **Text window**. The two remaining models are three-dimensional. Ignore the wire-frame model for the time-being, and select the **Space-filling item**. Of all the models, the space-filling model best simulates reality; it plots the arrangement of atoms in the molecule, using true atomic radii and bond distances.

Any three-dimensional model can be rotated, thereby revealing the molecule's shape in its entirety. Rotations can be achieved with the mouse or the keyboard. Try using the mouse first, as follows. Position the pointer somewhere in the **Model window**. The "arrow" (the pointer) becomes a "hand," indicating that the model can be rotated. Hold down the mouse button so as to "grab" the model with the hand, and then drag the mouse. The particular rotation that has occurred was determined by where the model was grabbed and by how the mouse was dragged. Take a moment to experiment with other rotations, using the mouse. Now try using the keyboard to produce similar kinds of rotations, as follows. Press the **Up Arrow key** several times. A rotation has occurred about the x-axis. Try pressing the other **Arrow keys** as well, and observe the similar types of rotations that occur. Finally, hold down the **Shift key**, and then press any one of the **Arrow keys**. The model is now rotating freely about a principal axis. Stop the animation by pressing any **Arrow key** or by clicking in the **Model window**.

A number of "settings" are available, which allow the display of three-dimensional models to be customized. Pull down the **Model menu**, and select the **3-D Settings item**. This opens the **3-D Settings dialog window**, which contains the controls for the various model settings. Two frames of reference can be included in three-dimensional model displays, these being the virtual sphere and the xyz-axes. Find the **Show Virtual Sphere check box** in the window. The check box is "checked" (i.e., there is an "x" in the box), meaning that the virtual sphere will be present in all three-dimensional model displays. The virtual sphere is, for instance, included in the display of the current space-filling model. Click on the **Show Virtual Sphere check box**. This disables (or "hides") the virtual sphere. The check box is no longer checked. Find the **Show xyz-Axes check box**. Disable this setting in the same way. Click on the **OK button** to make all of the changes take effect. The virtual sphere and the xyz-axes are no longer in the display. One advantage of not including these frames of reference is that rotations will operate with greater speed.

Another three-dimensional model setting is "Fill." The "fill" of a model refers to how the structure is rendered. The default fill is "shaded." The other available fills are transparent, solid and coloured. Open the **3-D Settings dialog window** and find the four "radio buttons" under the heading "Fill." Click on the **Transparent Radio button**. Click on the **OK button**. The atoms of the space-filling model are now transparent. Try rotating the molecule to fully appreciate the difference. Try using the two remaining fills, solid and coloured.

The final three-dimensional model setting is "Shape." A molecule's shape is classified by its molecular geometry (i.e., by its bonding pair arrangement) and by its electron pair arrangement. Molecular geometry is a subset of electron pair arrangement. The default shape is "molecular geometry." Notice that the model emphasizes the "angular" geometry of the water molecule. Open the **3-D Settings dialog window** and find the two radio buttons under the heading "Shape." Click on the **Electron Pair Arrangement radio button**. Click on the **OK**

button. The emphasis of shape in the model has changed. The model now emphasizes the "tetrahedral" shape of the water molecule (though its angular shape can still be discerned from within). The difference is that lone pairs are now represented as visual objects (grey spheres), whereas with the previous setting (molecular geometry), only the distortion they caused was a part of the display.

The wire-frame model is the final model to be selected. Pull down the **Model menu,** and select the **Wire-frame item**. The wire-frame model plots bond distances as line segments. It provides a good illustration of the geometric facets that comprise the molecule. Notice that the rotations of the previous space-filling model have been preserved. Rotate the wire-frame model to explore the molecule more completely.

Experiment with the three other volume-fills by selecting them from the **3-D Settings dialog window**. This completes the modelling process for water.

Click on the **Clear button** in the **Formula window**. This clears the formula and its accompanying displays. Now that the tutorial for water is complete, try building other molecules in the same way. The Fundamental Structures reference chart may be of assistance, particularly to someone who is not familiar with chemistry and/or VSEPR theory. The chart supplies one example molecule for each of the possible geometries.

FUNDAMENTAL STRUCTURES

EP = Electron Pairs
BP = Bonded Pairs
LP = Lone Pairs

GEOMETRIC ORIENTATION (EP)	MOLECULAR GEOMETRY (BP, LP)	VSEPR NOTATION	EXAMPLE FORMULA
Linear (1)	Linear (1, 0)	A_2	**H_2**
Linear (2)	Linear (2, 0)	AX_2	**BeH_2**
	Linear (1, 1)	AXE	**CO**
Trigonal Planar (3)	Trigonal Planar (3, 0)	AX_3	**BF_3**
	Angular (2, 1)	AX_2E	**SO_2**
	Linear (1, 2)	AXE_2	**O_2**
Tetrahedral (4)	Tetrahedral (4, 0)	AX_4	**CH_4**
	Trigonal Pyramidal (3, 1)	AX_3E	**NH_3**
	Angular (2, 2)	AX_2E_2	**H_2O**
	Linear (1, 3)	AXE_3	**HCl**
Trigonal Bipyramidal (5)	Trigonal Bipyramidal (5, 0)	AX_5	**PCl_5**
	Irregular Tetrahedral (4, 1)	AX_4E	**SF_4**
	T-Shaped (3, 2)	AX_3E_2	**ClF_3**
	Linear (2, 3)	AX_2E_3	**XeF_2**
Octahedral (6)	Octahedral (6, 0)	AX_6	**SF_6**
	Square Pyramidal (5, 1)	AX_5E	**BrF_5**
	Square Planar (4, 2)	AX_4E_2	**XeF_4**

FORMULA WINDOW

The **Formula window** contains a number of buttons, which are used to define the formula. These buttons include a collection of **Element buttons**, which together form a subset of the Periodic Table of the Elements. The reduced table only contains buttons for elements that are involved in VSEPR-type bonding (i.e., non-metals, metalloids, noble gases and beryllium, the one metal that partakes in covalent bonding). The buttons on the table also include a **Clear button**, **Plus** and **Minus Ion buttons** and a **Model button**. In addition to these buttons, the **Formula window** contains a display line, in which the formula appears as it is being defined.

Element Buttons

The **Element buttons** are found in the **Formula window**.

The **Element buttons** are used when defining a formula. A formula is defined by selecting the appropriate number of atoms for each element to be included in the formula. Selections are made by clicking with the mouse button on the desired **Element buttons**. Each click on an **Element button** inserts one atom of that element into the formula.

Atoms can also be deleted from the formula by clicking on the appropriate **Element button**, while holding down the **Shift key**.

The elements of the desired formula do not have to be entered in any particular order. For example, the formula for ammonia can be defined either as NH_3 or as H_3N. The latter nomenclature is incorrect, but VSEPRplex will still recognize the formula.

Important: VSEPRplex permits exploration of the vast majority of molecules that are predicted by VSEPR theory. See the Fundamental Structures reference chart for a list of just some of the molecules predicted by this theory.

Ion Buttons

The two **Ion buttons** are found in the **Formula window**.

The **Ion buttons** are used to "ionize" (charge) a molecule. Each click on the **Positive Ion button** increments the charge applied to the formula by one, by removing a valence electron from the molecule. Each click on the **Negative Ion button** decrements the charge by one, by adding a valence electron.

A formula can be ionized even if there are atoms still to be added. For example, if the formula to be defined is NH4+1 (the ammonium ion), the ionization does not have to be performed last. For example, the charge of +1 can be applied to the one atom of nitrogen, and when the four atoms of hydrogen are inserted, the charge will be applied to the finished molecule as a whole.

Model Button

The **Model button** is found in the **Formula window**.

The **Model button** is used to indicate that a formula is finished, and to have VSEPRplex determine whether the formula describes a molecule that is predicted by VSEPR theory. When the **Model button** is selected, the program will either accept or reject the formula, depending on whether the elements in their given quantities bond.

If the formula is accepted, a series of structural calculations are performed, the results of which are then displayed in the **Text window**. As well, a skeletal model is displayed in the **Model window**.

If, on the other hand, the formula is not accepted, the **Invalid Formula dialog window** opens. The window displays problem and solution messages. The problem message explains why bonding did not occur. The solution message suggests a general remedy and, in many cases, offers a working example formula, based on the attempted formula.

Clear Button

The **Clear button** is found in the **Formula window**.

The **Clear button** is used to erase the present formula in order that a new formula can be defined. When the **Clear button** is selected, all formula-related displays (e.g., the formula display line, the **Text** and **Model windows**, etc.) are cleared.

TEXT WINDOW

The **Text window** is simply the window in which texts, pertaining to the formula, are displayed. Text displays are accessible from the **Text menu**. The available texts are Element Attributes and Structural Calculations. For more information, see Text Menu.

MODEL WINDOW

The **Model window** is the window in which models of the molecule are displayed. Model displays are accessible from the **Model menu**. The available models are Skeletal, Lewis, Wire-frame and Space-filling. For more information, see Model Menu.

Rotations

Real-time rotations can be performed on any three-dimensional model, so as to better explore the molecule's shape. In the **Model window**, the molecule is encased in an imaginary glass sphere, called the "virtual sphere." Rotations are achieved by "rolling" the virtual sphere using the mouse or the keyboard.

When using the mouse, rotations are achieved by clicking (and holding down) the mouse button anywhere in the **Model window**, and by then dragging the mouse. The nature of the rotation is determined by where in the **Model window** the mouse button is initially clicked, and by how the mouse is then dragged. A rotation about the x-axis is acheved by clicking at the centre of the virtual sphere, and by then dragging the mouse up or down (along the y-axis). Similarly, a rotation about the y-axis is achieved by clicking at the centre of the sphere, and by then dragging the mouse left or right (along the x-axis). A rotation about the z-axis is achieved by clicking somewhere outside of the sphere (but still within the **Model window**), and by then dragging the mouse around the sphere. Any different rolling motions produce rotations about axes other than the principal three.

When using the keyboard, rotations are achieved by pressing any of the four **Arrow keys**. The **Up** and **Down Arrow keys** produce rotations about the x-axis. The **Left** and **Right Arrow keys** produce rotations about the y-axis. As well, a continuous rotation is achieved by holding down the **Shift key**, and by then pressing any of the **Arrow keys**.

3-D SETTINGS DIALOG WINDOW

The **3-D Settings dialog window** contains a number of controls (radio buttons and check boxes), which are used to modify and enhance the appearance of three-dimensional models. The control groups in the window are Shape, Fill and Environment.

Shape

The shape of a molecule is classified by the electron pair arrangement of the molecule and by its molecular geometry. For example, the electron pair arrangement of H_2O is tetrahedral, and the molecular geometry is angular. Electron pair arrangement is determined by the distribution of valence shell electron pairs in the molecule. Molecular geometry is determined by the electron pair arrangement, and by the number of bonded pairs in the molecule.

The **Shape radio buttons** are used to select which classification of shape is to be emphasized in the model. If the **Electron Pair Arrangement radio button** is selected, any lone pairs in the molecule are shown, so as to emphasize the electron pair arrangement of the molecule. If, instead, the **Molecular Geometry radio button** is selected, lone pairs are hidden, so as to emphasize molecular geometry.

Fill

The **Fill radio buttons** are used to change the rendering of the three-dimensional models. If the **Transparent radio button** is selected, the atoms of the molecule are displayed as spherical outlines. All parts of the molecule can be viewed at once, including any atoms that would normally be obscured from sight. If the **Solid radio button** is selected, all of the atoms are displayed as opaque, black spheres. If the **Coloured radio button** is selected, the atoms are displayed as opaque spheres, but they receive distinguishing colours. Finally, if the **Shaded radio button** is selected, the model is exposed to a light source.

Environment

The **Environment check boxes** are used to determine which frames of reference, if any, are to appear in the model display.

If the **Show Virtual Sphere check box** is checked, the virtual sphere is included in the model display. If the check box is unchecked, the sphere is not included. Since a model is rotated by clicking somewhere relative to the virtual sphere, it will often be useful to include the sphere.

If the **Show xyz-Axes check box** is checked, the xyz-axes are included in the model display. If the check box is unchecked, the axes are not included. It may be helpful to include the axes when the shape of the molecule is complicated and/or while rotations are being performed. Note: The z-axis is perpendicular to the x and y axes (and to the screen), and so the axis appears as a point at their intersection.

MENU BAR

The **Menu bar** is the strip of words across the top of the screen. The words identify the following menus: **File**, **Edit**, **Text**, **Model** and **Window**. Each of these menus contains a set of items. Each item, when selected, carries out a designated task.

A menu is opened (revealing the contained items) by clicking, and holding on the menu title. A particular menu item is selected by dragging the mouse over that item, and then releasing the mouse button. As soon as an item is selected, its function is carried out. Note: Items can only be selected when they are enabled.

Alternatively, menu items can be selected with the keyboard. For example, the element attributes of the formula can be displayed by pressing **Ctrl+E** (i.e., by holding down the **Ctrl key**, and then pressing the **E key**). There are many other keyboard shortcuts, each of which is indicated in the particular menu item title. For a complete list of shortcuts, see **Keyboard Shortcuts**.

File Menu

The **File menu** contains the following items: **Close Window**, **Export Window...**, **Page Setup...**, **Print Window...** and **Quit**.

The **Close Window item** is used to close the active window, if possible.

The **Export Window... item** is used to save the contents of the active window to a file as a picture in PICT format.

The **Page Setup... item** is used to initialize the printer.

The **Print Window... item** is used to print the contents of the active window.

The **Quit item** is used to quit VSEPRplex.

Edit Menu

The **Edit menu** contains the following items: **Undo**, **Cut**, **Copy**, **Paste**, **Clear**, **Select All** and **Show/Hide Clipboard**. These items are used to transfer information (text and pictures) between VSEPRplex and other applications.

The **Undo item** undoes the last user action.

The **Cut item** cuts the selected text or graphics. The information that is cut is removed and temporarily placed on the Clipboard.

The **Copy item** is used to copy the contents of the current selection to the Clipboard.

The **Paste item** places the contents of the Clipboard at the location of the insertion point (or in place of the current selection).

The **Clear item** removes the selected text or graphics without storing it on the Clipboard.

The **Select All item** is used to select all selectable objects in the active window.

The **Show/Hide Clipboard item** opens and closes the Clipboard window.

Text Menu

The **Text menu** contains the **Element Attributes item** and the **Structural Calculations item**. These items are used to display texts about the formula in the **Text window**.

The **Element Attributes item** is used to display the element attributes for each of the elements in the formula. The element attributes are the constant values used by the program when it determines the shape of the molecule. The display is particularly useful when performing similar calculations by hand.

The attributes that may appear in the display are as follows.

Symbol: Element abbreviation.

Name: Element name.

Atomic Number: Number of protons in the nucleus of an atom.

Covalent Radius: Radius of an atom when it partakes in a covalent bond.

Group: Column of the periodic table in which the element is found.

Covalence: Number of electrons that an atom can share with other atoms.

The **Structural Calculations item** is used to display a breakdown of the results of the calculations performed by the program when it determined the shape of the molecule. The display suggests why, according to VSEPR theory, the atoms of the particular molecule bonded as they did. The display is particularly useful when verifying any calculations completed by hand.

Note: Structural calculations are automatically displayed when a formula is successfully modelled.

The calculations that may appear in the display are as follows.

Molecular Formula: Formula that shows the number and types of atoms present in a molecule, but not the arrangement of the atoms.

Systematic Name: Name of a molecule under the Prefix system of nomenclature.

Common Name: Most familiar name by which a molecule is known (e.g., "water" for H_2O).

Central Atom: Atom to which the greatest number of bonds are formed in a molecule.

Valence Electrons: Number of electrons in all valence shells in a molecule.

Total Electrons: Number of electrons in all atoms in a molecule.

Bonded Pairs: Number of pairs of valence electrons involved in bond formation in a molecule.

Lone Pairs: Number of pairs of valence electrons not involved in bond formation in a molecule.

Electron Pairs: Combined number of bonded pairs and lone pairs in a molecule.

Single Bonds: Number of bonds in a molecule in which one electron pair is shared between two atoms.

Double Bonds: Number of bonds in a molecule in which two electron pairs are shared between two atoms.

Triple Bonds: Number of bonds in a molecule in which three electron pairs are shared between two atoms.

XAX Bond Angle: Angle formed by two adjacent central-terminal bonds (AX) that converge at a common central atom (A).

EP Arrangement: Shape of a molecule as determined by the geometrical distribution of valence shell electron pairs.

Molecular Geometry: Shape of a molecule as determined by its electron pair arrangement, and by the number of bonded pairs in the molecule.

VSEPR Notation: Notation for a formula, showing the number of central atoms (An), terminal atoms (Xn) and lone pairs (En) in the molecule.

Model Menu

The **Model menu** contains the following items: **Skeletal**, **Lewis**, **Wire-frame**, **Space-filling** and **3-D Settings**. The first four of these items are used to display models of the molecule in the **Model window**. The skeletal and Lewis models are two-dimensional. The wire-frame and space-filling models are three-dimensional. The **3-D settings item** is used to modify and enhance the appearance of three-dimensional models.

The models become progressively more advanced, and so it may be a good idea to view them in the order in which their items appear in the **Models menu**.

The **Skeletal item** is used to display a skeletal model, the simplest of the two-dimensional models. A skeletal model consists of a symmetrical arrangement of terminal element symbol(s) about the central element symbol. The model shows the "connectivity" of the molecule (i.e., which atoms are bonded together), but does not reveal the type(s) of bonds (single, double and/or triple, as the case may be), the bond angles or any lone pairs in the molecule.

The **Lewis item** is used to display a two-dimensional Lewis model. A Lewis model builds upon the skeletal model by showing the types of bonds (single, double and/or triple) and the lone pairs in the molecule.

The **Wire-frame item** is used to display a three-dimensional wire-frame model. A wire-frame model displays the molecule as a collection of line segments, which represent the distances between atoms. The line segments connect all of the atoms in the molecule to one another, regardless of whether they are bonded. Bond distances are scaled to reflect the true proportions of the molecule, and also to suggest linear perspective. A wire-frame model nicely illustrates the geometrical facets of the molecule, and is most helpful in demonstrating the classification of shape. For more information on shape, see Shape.

The **Space-filling item** is used to display a three-dimensional space-filling model. A space-filling model displays the molecule as an assembly of spheres, which represent the atoms in the molecule. Bond distances and the covalent radii of the atoms are scaled to reflect the true proportions of the molecule, and also to suggest linear perspective. A space-filling model provides a good example of the theoretical appearance of the molecule.

The **3-D Settings item** is used to open the **3-D Settings dialog window**. The **3-D Settings dialog window** permits the appearance of three-dimensional models to be modified and enhanced in a number of ways. For more information, see 3-D Settings Dialog Window.

Window Menu

The **Window menu** contains the following items: **Default Positions**, **Formula**, **Text** and **Model**.

The **Default Positions item** is used to reset all open windows to their default positions and sizes.

The **Formula**, **Text** and **Model items** indicate which windows are currently open, and are used to select which of the windows is active. A window is open if its corresponding item in the **Window menu** is enabled. The active window is the window whose item has a check mark. A different window can be activated by selecting its corresponding menu item.

KEYBOARD SHORTCUTS

MENU ITEM	KEYBOARD SHORTCUT
File	
Close **W**indow	Command+W
Export Window...	none
Page Setup...	none
Print Window	none
Quit	Command+Q
Edit	
Undo	Command+Z
Cut	Command+X
Copy	Command+C
Paste	Command+V
Clear	none
Select **A**ll	Command+A
Show/Hide Clipboard	none
Text	
Element Attributes	Command+E
Structural **C**alculations	Command+C
Model	
Skeletal	Command+S
Lewis	Command+L
Wire-f**r**ame	Command+R
Space-**f**illing	Command+F
3-**D** Settings...	Command+D
Window	
Default Positions	Command+0
Formula	Command+1
Text	Command+2
Model	Command+3

CHEMISTRY

Bruckman, Herman J., et. al. Understanding Chemistry, Toronto, Ontario, 1988.

Cotton, F. Albert, et. al. Advanced Inorganic Chemistry: A Comprehensive Text, U.S.A., 1962.

Cotton, F. Albert, et. al. Chemistry An Investigative Approach, Boston, Massachusetts, 1973.

Gillespie, Ronald J., et. al. Atoms, Molecules, and Reactions: An Introduction to Chemistry, Englewood Cliffs, New Jersey, 1994.

Gray, Harry B. Electrons and Chemical Bonding, New York, New York, 1965.

Petrucci, Ralph H., et. al. General Chemistry with Qualitative Analysis, 2nd ed., New York, New York, 1987.

Sanderson, R. T. Inorganic Chemistry, New York, New York, 1967.

Siebring, B. Richard Chemistry, London, England, 1967.

Stranks, D. R. Chemistry A Structural View, Cambridge, England, 1966.

COMPUTER SCIENCE

Chen, Michael, et. al. A Study in Interactive 3-D Rotations Using 2-D Control Devices. Computer Graphics. Vol. 22, No. 4 (1988): 121-129.