

**Chemical for Windows Version 1.4** is a molecular modeling program that constructs computer models of molecules. Atoms are selected from a Periodic Table that is presented when the Atom is selected from the Main Menu. Molecules are made by dragging one atom to meet another Atom. Motion of the Atoms and Molecules can be simulated by enabling Time. The minimum energy configuration can be found by enabling Minimize Energy. The Shade Main Menu options shades the image to enhance the three dimensional effect (a 256 color graphics board is required). The image generated can be transferred to a graphics program via the Windows Clipboard and editing and printing.

This program is an extension of Chemical (for DOS) which was written in Turbo PROLOG to run under DOS. This new version has been ported to Borland C++ to run under Windows 3.1.

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**Windows** - Chemical opens with four windows: Control, Message, Color and View. The window selection can be modified via the window selection the Main Menu that appears at the top of the screen.

**View Window** - This windows shows the molecular model as it is being built. The Scroll Bar around this window can be used to move the image vertically or horizontally. An option in the Main Menu will make the view window larger.

**Comment Window** - This window displays a list of comments about actions that have taken place in the View Window. Messages that have scrolled off the screen can be viewed via the vertical Scroll Bar. An option in the Main Menu modifies the comment window so that it will show the data file that is being created.

**Control Window** - This window contains controls that are used to change the view, rotate, enable features and set parameters for the atoms shown in the View Window.

**Color Window** - This window contains three Scroll Bars: RED, GREEN, and BLUE and a List Box. The atoms selected appear in the List Box. Selecting an Atom from the listbox will move the slider on the three scollbars to the RGB colors assigned to that atom. The color for the selected Atom can be changed by moving the Scroll Bars.

**Matter Window** - The window command from the Main Menu can be used to change the upper left hand window to the Matter Window. This window contains 15 buttons that will be used in future versions of this program.

**Zooming View Window** - Two Scroll Bars in the Control Window are used to change the field of view within the View Window. The larger Scroll Bar is for course adjustment and the smaller Scroll Bar is for fine adjustment.

**Mass/Density Window** - Enable the Mass/Density window to display the mass and density.

**View Selection Window** - Enable the View Selection window to change the view selection when the View Window is enlarged to full screen.

**Double Clicking Left Button with cursor in View Window** - Displays a Periodic Table from which Atoms can be selected.

**Single Clicking Left Button with cursor on an atom, without moving cursor** - Displays an Information box giving the position, mass, name, and orbital details of the selected atom. Pushing a button in the information box deletes the selected atom.

**Using Left Button to drag an unbound atom to another atom** - Bonds selected atom to target atom or molecule.

**Using Left Button to drag a bound atom to empty space** - Disconnects the atom from molecule. If the atom was bond to more than one other atom, moving it several times will disconnect all bonds.

**Using Left Button to drag a bound Atom** - Small adjustments to the location of a bound atom can be made by dragging the cursor within the selected atom.

**Using Right Button to drag a Molecule** - The right mouse button is used to move a molecule.

**Main Menu** - The Main Menu appears at the top of the screen.

**File** - Allows molecules to be saved to or read from the disk.

**Atom** - Displays a Periodic Table from which Atoms are selected.

**View** - Select the viewing direction: Front, Back, Right, Left To, or Bottom. Also, rotate the molecule up, down, left, or right.

**Control** - Used to change the Temperature, Time Step, or View Size.

**Window** - Changes the arrangement of windows on the screen.

**Selecting Atoms** - Select the atom menu from main menu at the top of the screen (or double click the left mouse button with the cursor in the view window). A Periodic Table will appear in a Dialog Box. As Atoms are selected they will appear in the List Box. Push the OK button after all desired atoms have been selected.

**Make Hybrid or Ions** - Clicking the mouse on an item in the hybrid or ion list will add that attribute to the Atom. The ListBox can be modified directly, if desired.

**Repeat** - The repeat button can be used to duplicate the previous selection.

**Manipulation of Atom and making Molecules** - After Atoms are selected and displayed in the View Window they can be manipulated via the mouse.

**Moving Atoms** - Placing the cursor on an Atom and pushing the left mouse button down will select the Atom to be moved. Move the cursor to the new position while holding down the mouse button.

**Bonding Atoms to make Molecules** - Moving an Atom to a position on top of another atom will bring up a Atomic Bonding Dialog Window. All possible ways these two atoms can be bound are list in a List Box. Pushing OK will bind the atoms using the selected bond.

**Moving Molecules** - Placing the cursor on a Molecule and pushing the right mouse button down will select the Molecule to be moved. Move the cursor to the new position while holding down the mouse button.

**Controlling the direction of Bonding** - Place the cursor on the side of the target Atom closest to the desired bond direction. The bond in this direction will be the highlighted in Atomic Bonding Window. Some ring structures require hybrids with a \_4, \_5 or a \_6 ending. The highlighted bond for these hybrids is the selection that will form a ring structure.

**Breaking an Atomic Bond** - Moving a bonded Atom more than 1.5 times its bonding distance will free the bond.

**Selecting a Molecule** - Pushing the left mouse button will select the molecule that the cursor is on. The rotation of an individual molecule requires that the molecule be selected.

## **Modifying how atoms are shown**

**Labeling Atom** - Atom will be labeled if the Label Check Box is enabled.

**Bond Lines** - Bond Lines will be enabled if the Bond Line Check Box is enabled. The width of the bond line corresponds to the bond number.

**Coloring Atom** - Use the main menu to place the Color Window in the upper left hand corner of the screen. The atoms selected appear in the List Box. Selecting an Atom from the listbox will move the slider on the three scollbars to the RGB colors assigned to that atom. The color for the selected Atom can be changed by moving the ScrollBars. The color for all atoms of this type will be changed.

## **Modifying the View**

**Top, Bottom, Right, Left, Front, Back** - Selecting one of these radio buttons in the Control Window will change the direction objects are viewed from.

**Rotate U,D,L,R** - Clicking on of these buttons with the "all" option selected will rotate all object by a small angle. The "select" option will only rotate the molecule selected.

**Screen Size Edit Box** - Making the value in the Screen Size edit box smaller reduces the screen size and makes the image larger. Therefore, pushing the "+" button will make the image smaller, and pushing the "-" button will make it bigger. A new value can be entered directly into the Screen Size Edit Box, however, the "+" or "-" button must be pushed for the change to take effect.



## **Time and Temperature**

Time and temperature are used to modify the dynamic motion of atoms when time is enabled.

**Time Checkbox** - Enabling the Time checkbox will cause the atoms to move. Atoms that come close together will bond together if bonding is possible.

**Time step Edit Box** - When Time is enabled the atoms are displayed at time intervals that are determined the Time Step. The time incremented or decemented via the "+" and "-" buttons next to the Time Step Edit Box. The time step can also be changed by direct entry into the Time StepBox, however, the "+" or "-" button must be pushed for the new value to take effect.

**Temperature Edit Box** - Changing the value in the Temperature Edit Box will change the kinetic energy will be given when they collide with the border or another atom. Use the "+" or "-" buttons to change the value.

**Motion simulation** provides a very simple model of the movement of atoms and molecules. Atoms move with a velocity that increases with temperature and decreases with mass. Atoms that make contact will be bonded together if possible. When atoms hit the side of the View Window that are reflected back. Making the View Window smaller will increase the probability of collisions.

**Initial Velocity** - Atom and Molecules are given an initial velocity that corresponds to their thermal Kinetic Energy

**Reflection** - Atoms are reflected off of the View Window walls and off of each other ( if they are not bonded)

**Bonding** - Atoms that collide bond, if possible.

**Energy** - Enable the Minimize Energy checkbox to randomly search for a lower energy position for the atoms. Each atom is tested to determine if a slight random movement in the X, Y, or Z direction results in a lower energy configuration. The random step size can be adjusted to speed up or slow down the search.

**Saving Files** - Use the Save or Save As option from the File menu item at the top of the screen. Two options are available to modify the format of the data written to the disk. One does not include empty orbitals and the other outputs an abridged format that only include location information.

### **File Format Options**

Exclude Empty Orbitals - This option excludes empty orbitals when writing the file.

Short Format - This option writes a shortened format that include only numbers.

**Compatibility with CHEMICAL and CHEMVIEW** - Although Chemical for Windows can read files from Chemical for DOS, the compatibility does not work in the other direction. A new version of CHEMVIEW, version 2.1 was written to show animation of molecules written with Chemical for Windows.

**Shading**

The shading option in the main menu adds 3D shading and shadows to the molecule. This option requires a Super VGA monitor with 256 colors. Windows must be set to a 256 color mode in order to use this option. Also, this shading is very computationally intensive and may take several minutes to draw an image.

An option in the shading menu saves the image to the Clipboard. This option copies the Palette to the Clipboard to maintain color integrity.

**Hydrogen Bonds**

A hydrogen bond is formed when two atoms share a common hydrogen atom. One of the atoms must be highly electronegative. This bond type can be formed by dragging an atom to meet a hydrogen atom that is attached to a highly electronegative atom such as Oxygen or Nitrogen.

### **Crystals (Ionic Structures)**

Selecting the Matter/Crystal option from the main menu displays a Dialog Box that can be used to construct 3D models of Ionic Structures. Ionic structures are built by selecting the ions that are used to build one unit cell. The size of the unit cell can be changed manually or the size can be computed by the program. The List Boxes are used to select the ions that will be used. The four List Boxes on the left are used to select the ions for the center, corner, face, and edge of the unit cell. The four List Boxes on the right are used to place ions at specified locations within the cell. The locations for the right hand list boxes are specified by filling in the location boxes above each list box. The location value can range from 0.0 to 1.0 and correspond to the ion location within the unit cell.

After the ions are selected and their locations within the unit cell are specified, the size of the unit cell can be approximated by pushing the size button. Pushing the OK button will display the crystal. The crystal structure can be modified by re-issuing the Matter/Crystal command. The Clear button on the Crystal Dialog Box clears all ion selections.

In addition to **Chemical for Windows**, the following programs are available. All are for IBM PC and compatibles.

**CHEMICAL Ver 4.2 for DOS** is a molecular modeling program that uses a menu selection interface. This program does not provide all of the features of Chemical for Windows. This program will probably not be extended past version 4.2. Requires a graphics monitor.

**CRYSTAL Ver 1.0 for DOS** is used to build crystal structures. English commands are used to describe the structure. The easiest way to build a new structure is to start with a similar structure. The necessary changes can then be made using the built in editor. Requires EGA/VGA.

**CHEMVIEW Ver 2.0 for DOS** is a companion program that shows 3-dimensional animation of the models generated with CHEMICAL. Requires EGA or VGA monitor.

**BIOCHEM Ver 1.0 for DOS** combines molecules made with Chemical into large molecules. The attachments can be made using covalent, hydrogen, double hydrogen, peptide, or ionic bonding. Files for common biochemical molecules are included. CHEMICAL data files have the extension .DAT. Files that are combined using BioCHEM have the extension .BIO. Biochem requires a CGA or EGA monitor.

**PLANETS Ver. 4.1 for DOS** computes information relating to the position, distance, magnitude, orbit view, skyview, etc for the major planets, four minor planets or Halley's comet on a specified date and time. Planets works with CGA, EGA, Hercules, or VGA monitors.

All of these programs are public domain and updates can be obtained from the various Public Domain / Shareware distributors. If you would like to receive the latest version directly from the author the price list is listed below. Updates, for people that received their current version from the author are half price. Please indicate if you want 3 1/2 or 5 1/4 inch disks.

CHEMICAL for Windows without source code	\$20
CHEMICAL for Windows with source code	\$30
CHEMICAL/CHEMVIEW/CRYSTAL/BioCHEM for DOS	\$20 for set
CHEMICAL/CHEMVIEW/CRYSTAL/BioChem with source code	\$30
Planet Version 4.1 with Pascal source code	\$10
Overseas shipping (please, check drawn on US bank or cash)	\$5

Larry Puhl  
6 Plum Court  
Sleepy Hollow, Ill. 60118



A Dialog Box is a temporary window that appears on the screen to request specific input.

Hybrids are combinations of atomic orbitals that define the directional characteristics of Atoms.

Ions are Atoms that have an electrical charge do to the addition or deletion of an electron.

A List Box lists the possible selections in a box from which the user can select an item.

Menu at the top of the screen.

A Scroll Bar is a horizontal or vertical control that is used to change the value of a variable or move the contents within a window.

