Molwin

The program MolWin reads a file with the atomic coordinates and display a molecule. It supports different input formats.

File
- Open

Edit
- Copy

View
- Stereo
- ZoomIn
- ZoomOut
- Center

Options
- Plot
- Chemistry
- Input
- Save

Help
- About

Tools bar
- It is located at the right side of the window.

Stereo

Show two stereo projections. To modify a stereo angle select Option | Color | Stereo Angle.

Zoom In

Increase the scale by 10%.

Zoom Out

Decree the scale by 10 %.

Center

Move the molecule to the center of the screen (approximately).

Color and plot options

Option	Description
Bond Width	A width of lines in pixels which used to show bonds.
Bond Color	A color for bonds.
Rotation Angle	An angle (in degrees) to rotate the molecule. Increase the angle if you want to speed up the animation.
Sphere Factor	A radius of the circle which represents an atom with the atomic number *n* is determined by the product of *SphereFactor* and Van-der-Waals Radius.

Switches	Description
Show Atoms	Display circles representing atoms.
Show Hydrogens	Display hydrogen atoms.
Show Bonds	Display bonds as sticks.
Label Atoms	Put atomic symbols or atom names (if input format allows them) near corresponding atoms.

Chemistry Options

Option	Description
BondFudge	see next option. The default value for BondFudge is 1.12 (see acknowledgment).
Atomic Number or Chemical Symbol	Select a chemical element for the following two fields.
Atomic Radius	For some input formats (XYZ) there is no connectivity information in the input file. Two atoms are considered to be connected if *D12 < (R1+R2)*BondFudge* , here *Ri* is an atomic radius of atom i and *D12* is a distance between atoms.
Van-der-Waals Radius	The radius of the circle which represents the atom is determined by *SphereFactor* Van-der-Waals radius*.

Initially boxes **Atomic Radius** and **Van-der-Waals Radius** are dimmed. Enter a correct atomic radius or chemical symbol and click **Radius** button. Now you could change both radius.

Input Options

Select input format. See File|Open.

Save Options

To save current options in the "molwin.ini" file. To reset to default options erase this file from your WINDOWS directory.

Edit | Copy

The Copy command places an exact copy of the plot window(s) in the Clipboard.
To paste the copied picture into any other program (PaintBrush, for example), choose Edit Paste.

File | Open

Read the file with the atomic data. It should be in one of the following formats:

XYZ, Gaussian Output, PDB

XYZ format (subset!)

A short description of the subset of XYZ format used by the program.

Line(s)	Description
1	*N*, a number of atoms .
2	a comment (ignored).
3...*N*+2	atomic coordinates, one line per atom (see below).

The line with the atomic coordinates has four fields in a free format.

Field(s)	Description
1	atomic number or chemical symbol of the element. Chemical symbol may be followed by an optional number without any space between the symbol and the number. (i.e "C1" but not "C 1").
2--4	x,y,z Cartesian coordinates.

GaussianOutput

The output file of the program GAUSSIAN 92 for Windows.

PDB format

The Brookhaven Protein Databank format.

Help | About MolWin

Show copyright and version information.

Tools Bar

Icon(s)	Description
X,Y,Z	Rotate a molecule about the selected axis. To start press the left or the right button for clockwise or counterclokwise rotation respectively. To stop rotation release the button. The speed of the rotation is detemined by a Rotation Angle.