MolWorks / Version 2.0 Manual

Welcome to MolWorks™

Releasing Version 2.0 on September 29, 2003

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[1] About MolWorks

MolWorks is a software tool for computer aided molecular design.

●Multi-platform support

MolWorks can be run on any platform running a Java™ VM (Virtual machine), such as Windows and Linux (Redhat).

●About modeling

MolWorks can build molecules by drawing them within the Builder Panel. MolWorks can handle 3D molecules. You can clean up molecules by using a simple minimization algorithm. You can easily change atom type and bond order for molecule. You can select Wire/Ball & Stick style. You can handle many molecules by using tab panels.

●Reading molecule files and output files of computational chemistry programs, and saved molecule files

MolWorks can read molecule files (XYZ Format File(*.xyz) & Protein Data Bank File(*.pdb) in Version 2.0) and display molecules within the Builder Panel. In addition, it can read input output files of Gaussian, GAMESS, MOPAC, and Q-Chem, and can analyze and visualize the results. MolWorks also can write molecule files (only XYZ Format File(*.xyz) in Version 2.0) and input files for the programs (see next).

●Pre and Post processors for quantum mechanics programs

MolWorks has interfaces for Q-Chem / Gaussian / GAMESS / MOPAC. MolWorks include a CNDO/2 calculation engine and can display the MO (Molecular Orbital) within the Builder Panel.

MolWorks can convert a Gaussian input data into a Q-Chem input data and create an input data file for Q-Chem.

MolWorks can submit a Gaussian job. (only when Gaussian program is installed locally.)

●Properties Estimation

MolWorks can estimate molecular properties using “Group Contribution Methods” and “Principle of Corresponding States”. You can estimate molecular properties and squeeze down the target molecule from the list. MolWorks can display diagram of “Equation of the State” for the molecular mixtures.

[2] System Requirements

Windows 98/2000/NT 4.0/XP (Pentium MMX 233MHz and above)
Linux (Redhat)

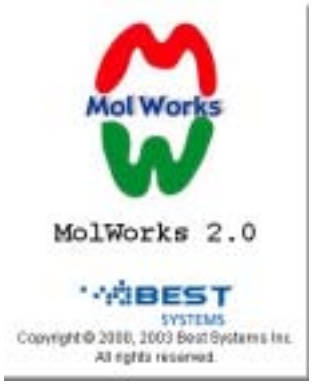
45MB hard disk space (including Java™ VM)
32MB RAM (64MB recommended)
256 color VGA monitor (800x600 or greater)
Ethernet Card or Ethernet Board is necessary.

[3] How To Start Up

●Windows Users
Execute the MolWorks from the "**Start Menu**".
●Linux Users
Execute the command **MolWorks** from the command line in the window.

While the **Startup Window is** displayed, several modules are loaded. Then **Initial Display** will be appeared on the screen.

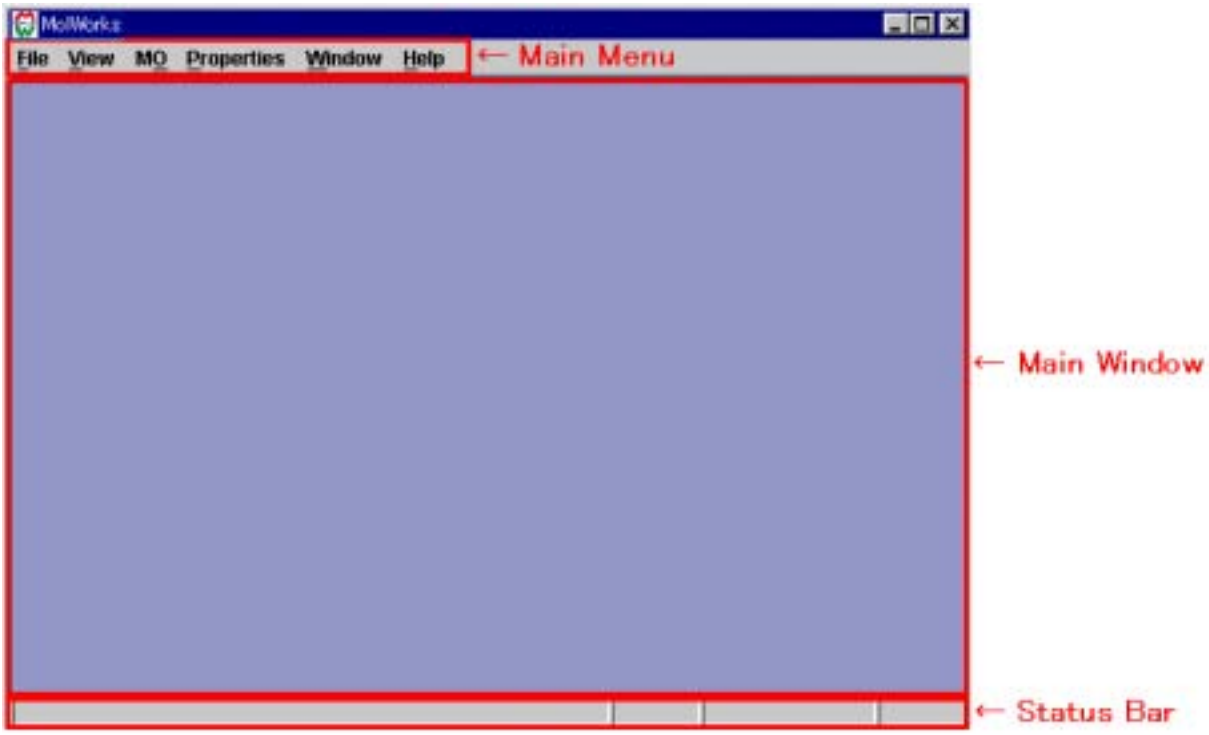
（**Startup Window**）



（**Initial Display**）

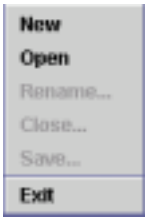
[4] Display Contents

The **Initial Display** consists of the **Main Menu** / **Main Window** / **Status Bar**.
（**Initial Display**）



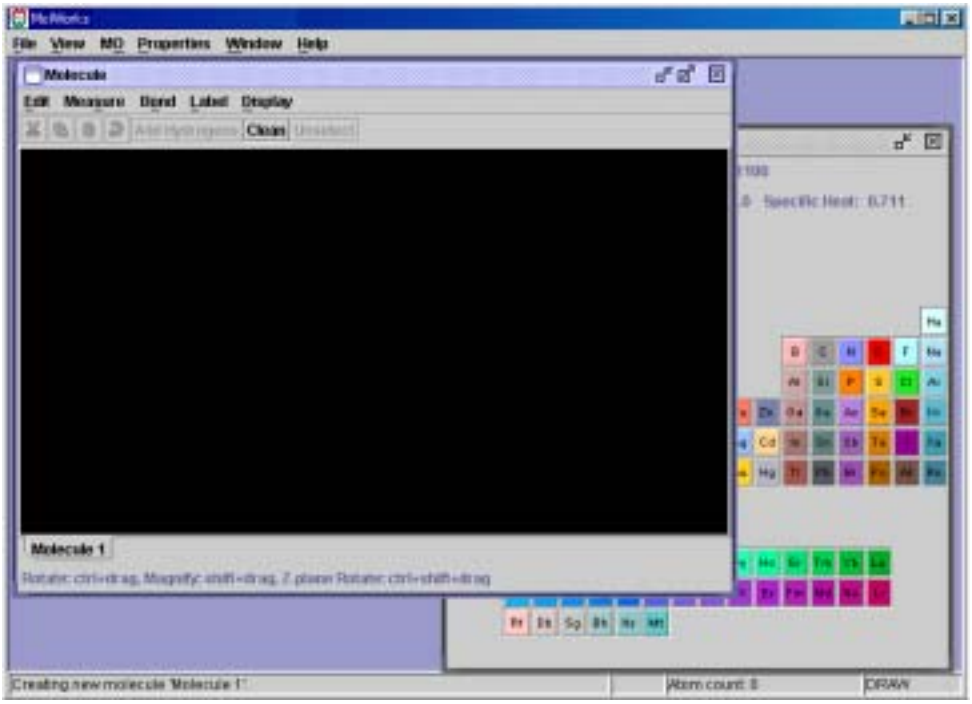
I. Main Menu

1) File



1)-a. New

In the case of the **Molecule Window** and **Periodic Table Window** are opened in the **Main Window**. If the **Molecule Window** is already displayed, new **Builder Panel** will be added.

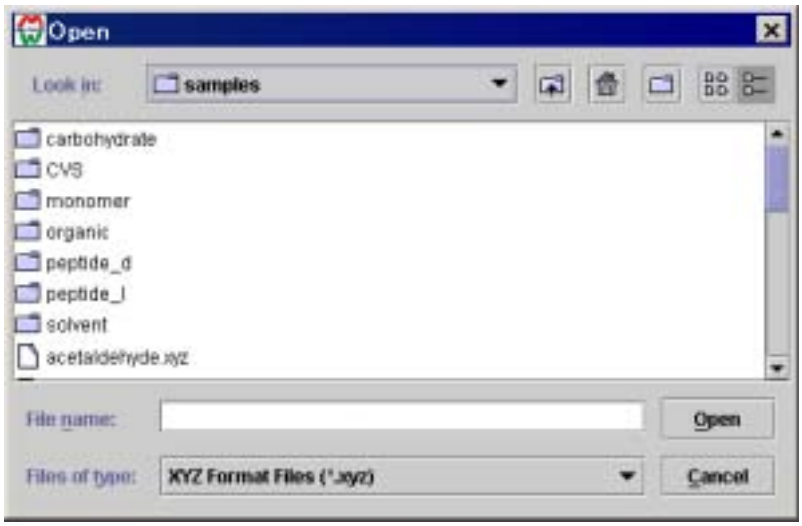


1)-b. Open…

The browser for open file will be appeared. Select a molecular coordinate file and press Open. The molecular structure will be displayed in the **Builder Panel**.

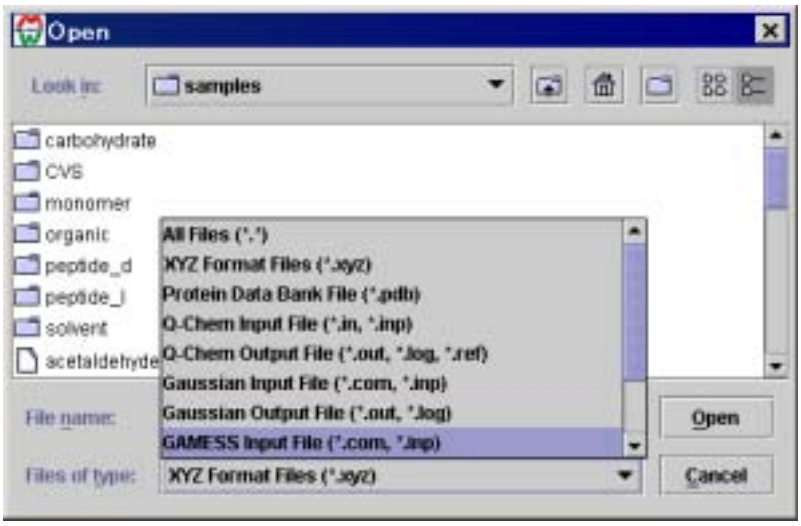
1)-b-1: File name

Display the selected file name.

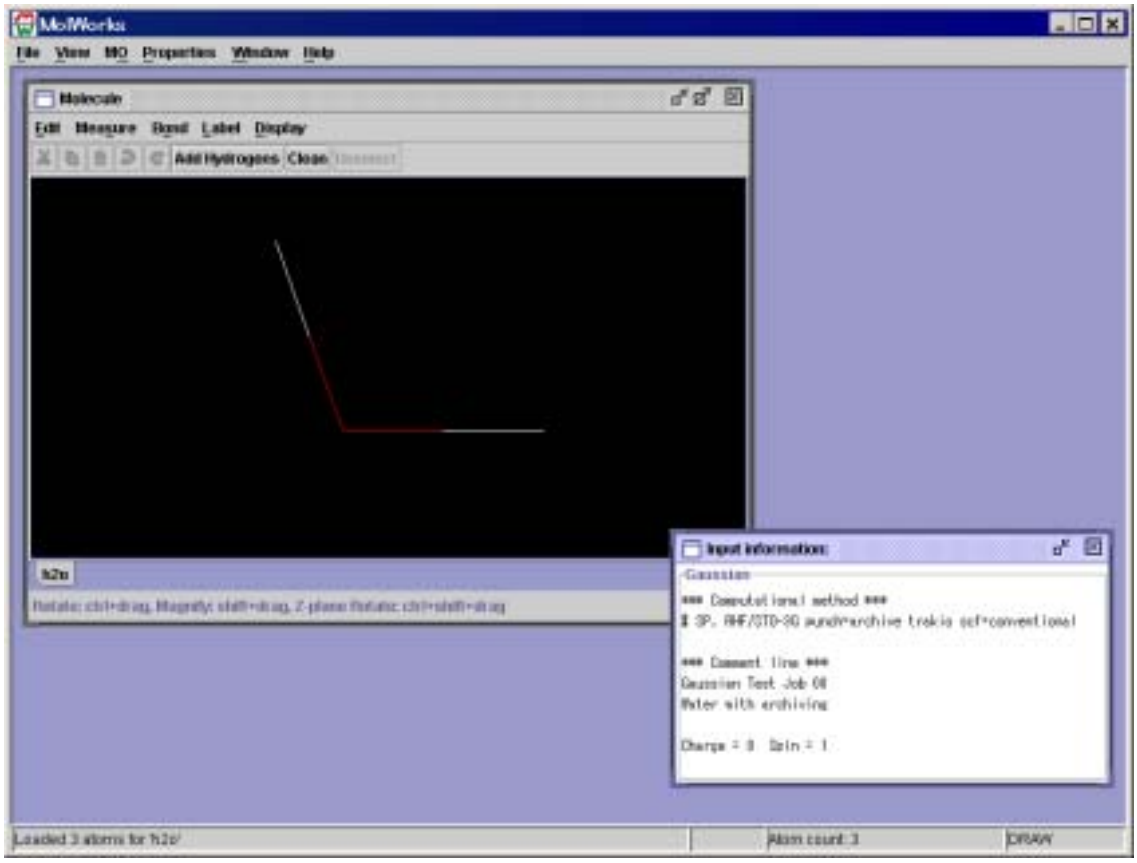


1)-b-2: Files of type

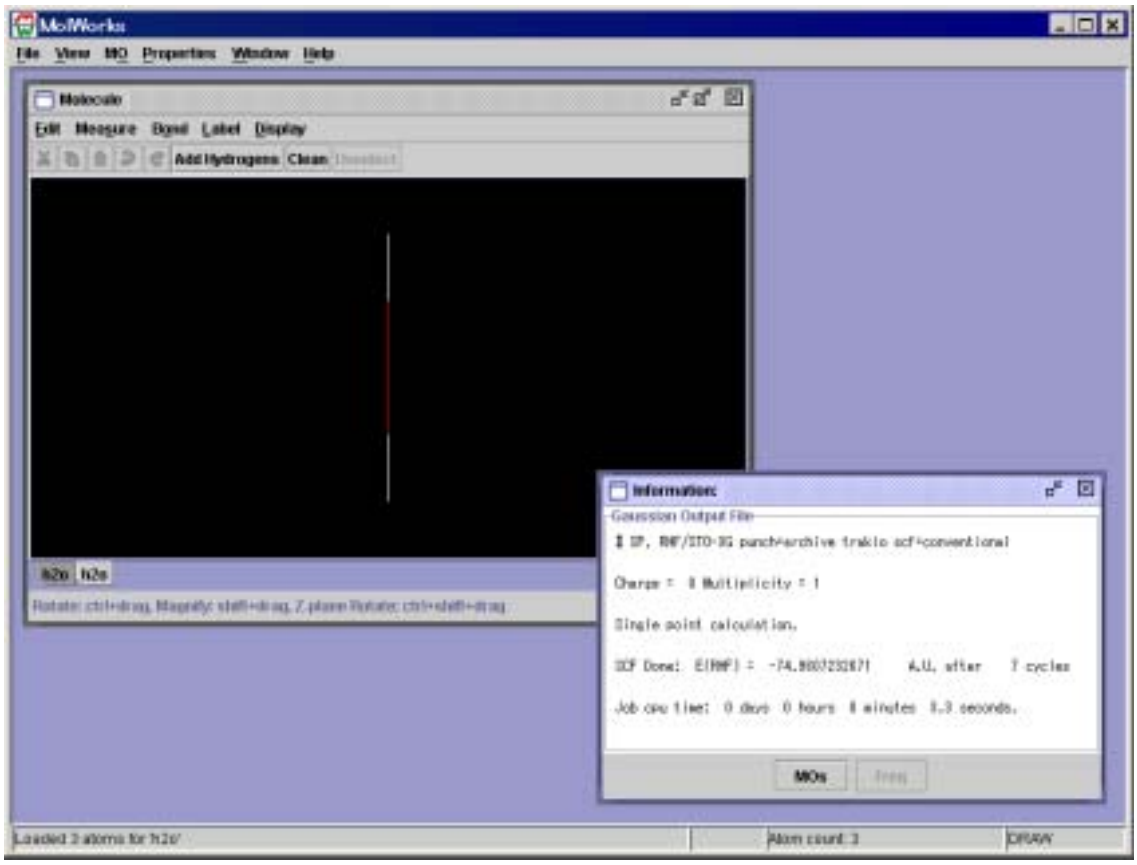
Specify the reading file type. In version 2.0, it can read XYZ Format File(*.xyz), Protein Data Bank File(*.pdb), and input and output files of Gaussian, GAMESS, MOPAC, and Q-Chem. When the input files are read, the molecular structure with the options and parameters for the calculation are displayed, and when the output files are read, the molecular structure with the results of calculation are displayed.



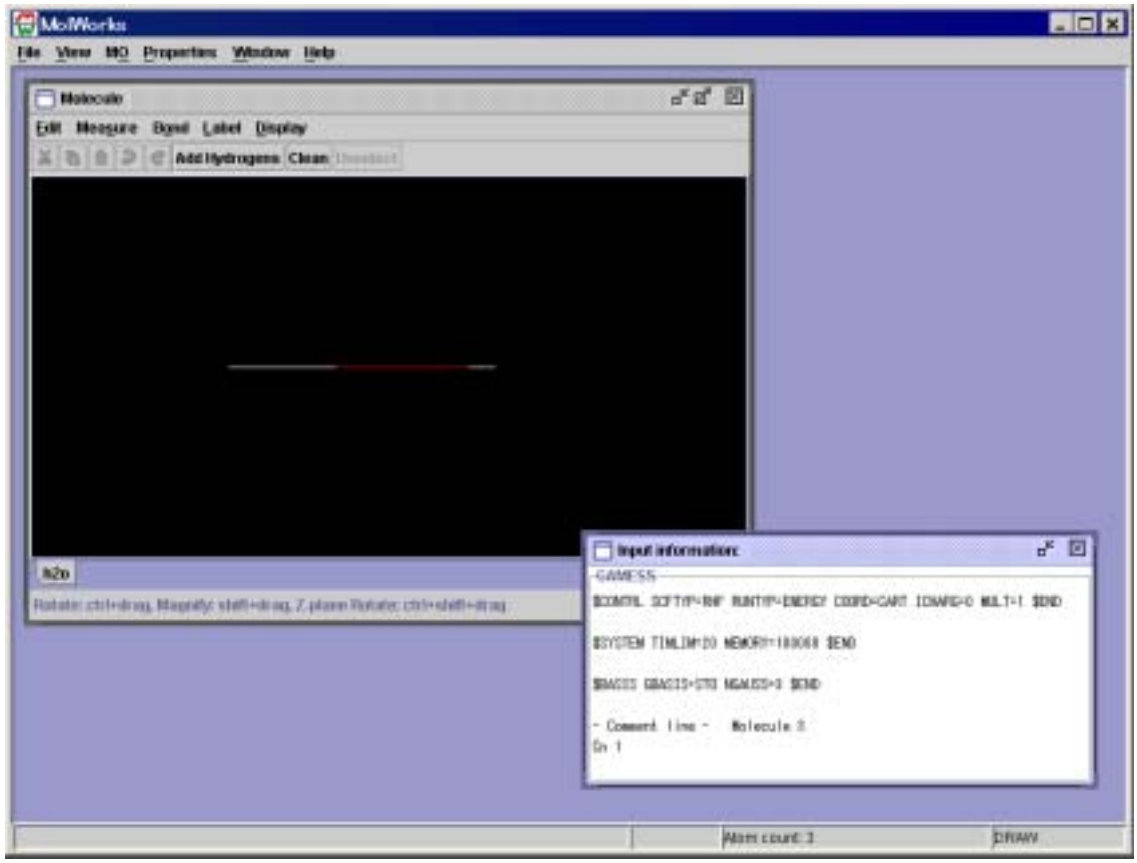
1)-b-3: In the case of reading Gaussian input file (h2o.com)



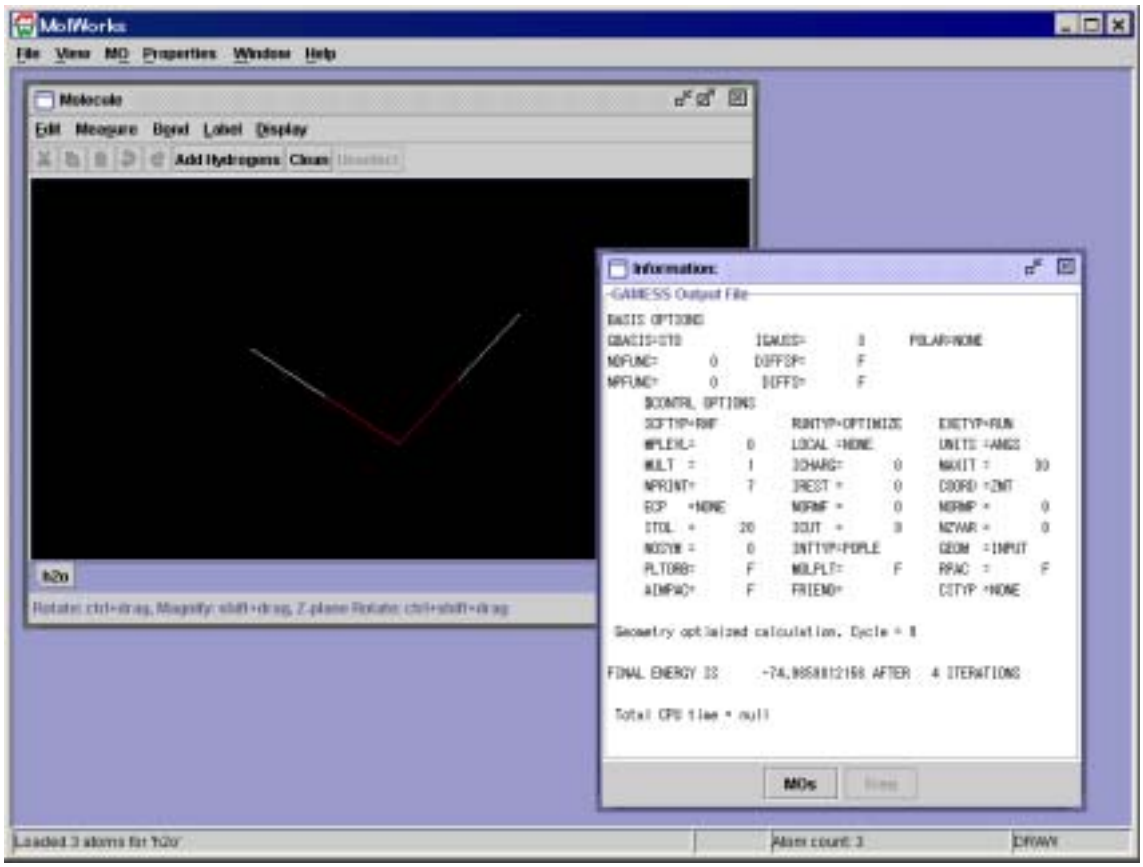
1)-b-4: In the case of reading Gaussian output file (h2o.log)



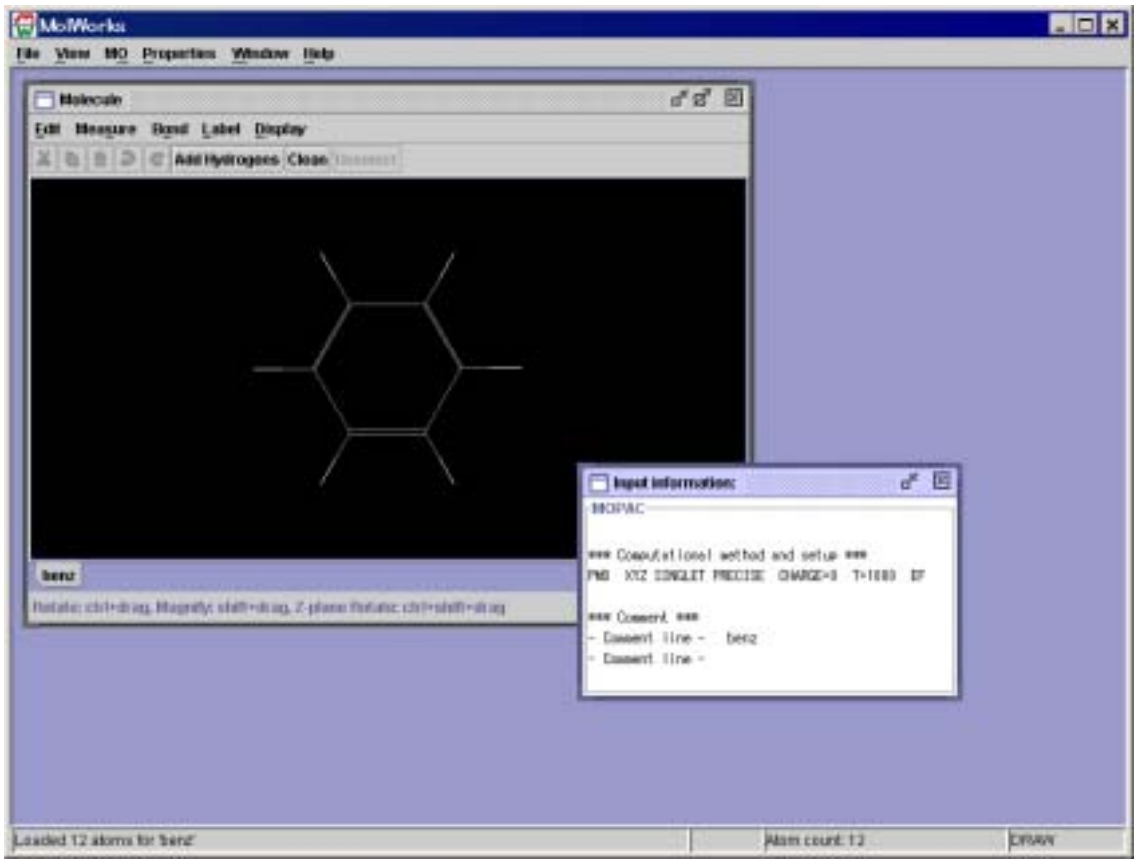
1)-b-5: In the case of reading GAMESS input file (h2o.inp)



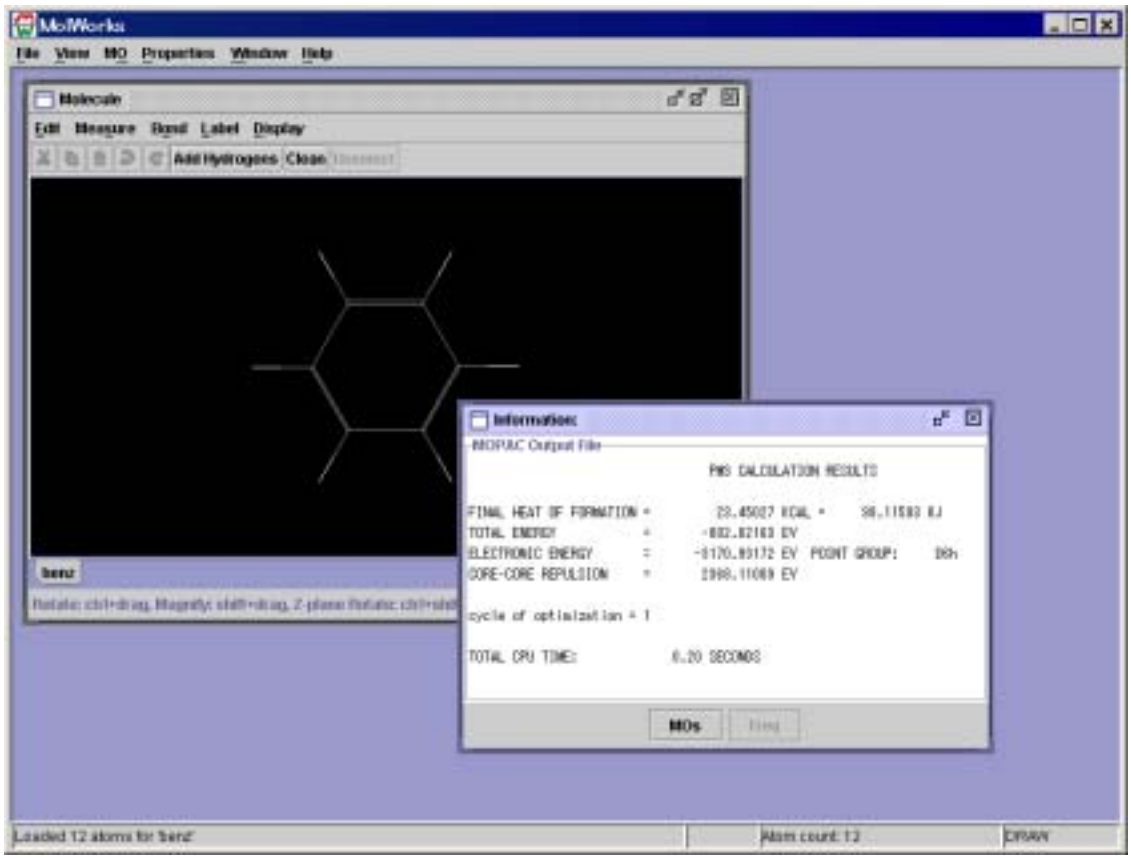
1)-b-6: In the case of reading GAMESS output file



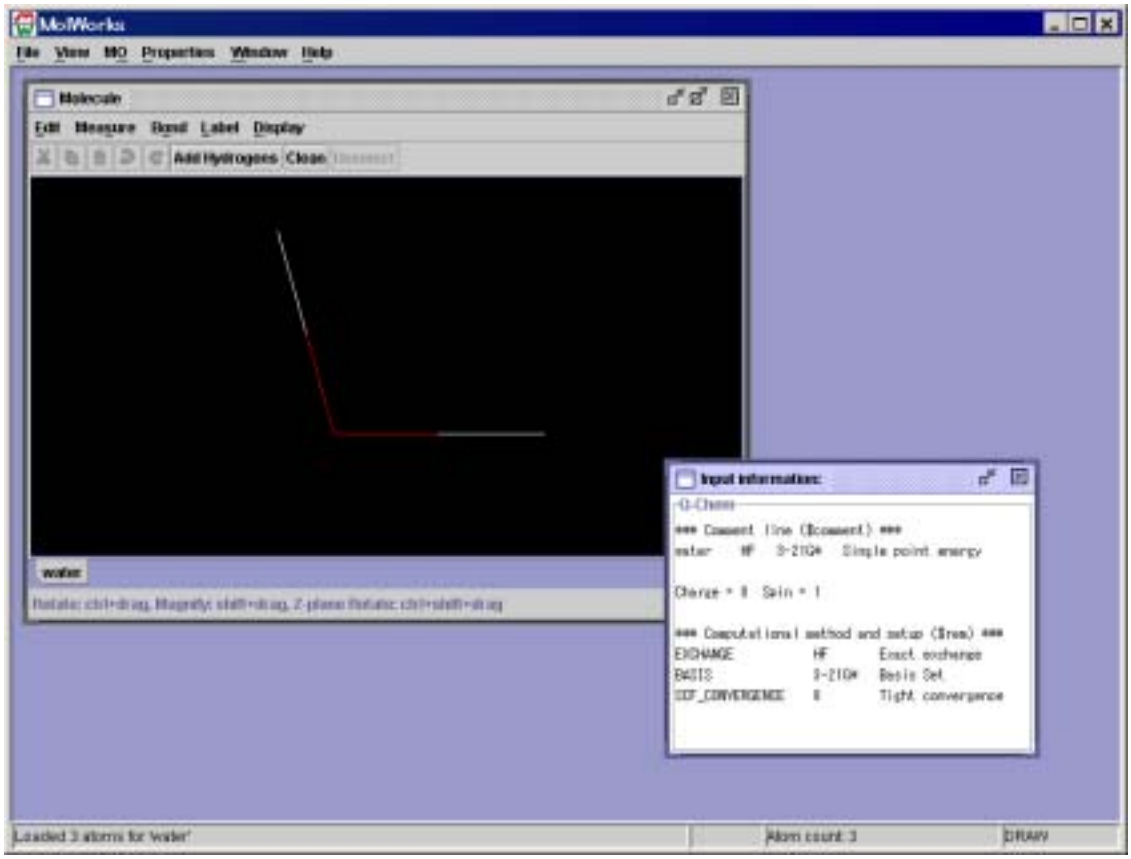
1)-b-7: In the case of reading MOPAC input file (benz.dat)



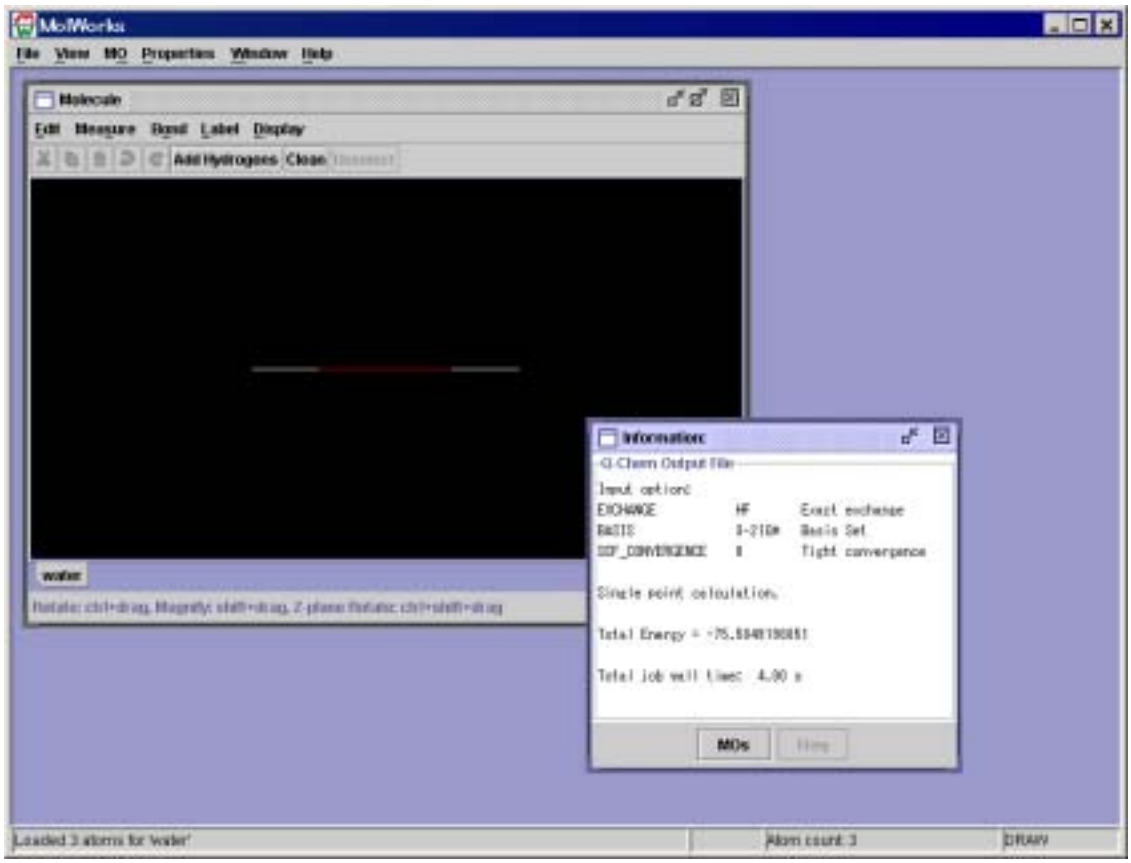
1)-b-8: In the case of reading MOPAC output file (benz.out)



1)-b-9: In the case of reading Q-Chem input file (water.in)



1)-b-10: In the case of reading Q-Chem output file (water.ref)

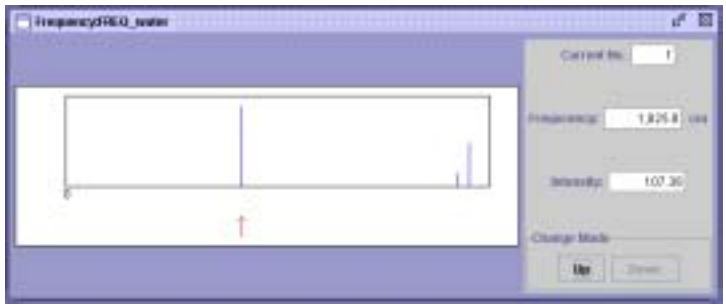


1)-b-11: The orbital energy level

The orbital energy level is displayed when the output files are read and the MOs button in the **Information Window** is pressed.

1)-b-12: Frequency

The spectrum of IR is displayed if the result of vibrational analysis is included in the output files and the Freq button in the **Information Window** is pressed.



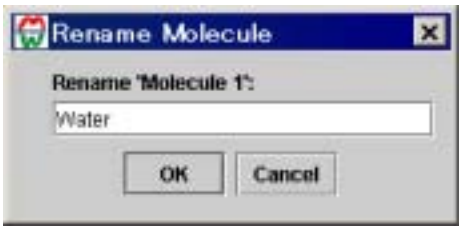
1)-c. Rename…

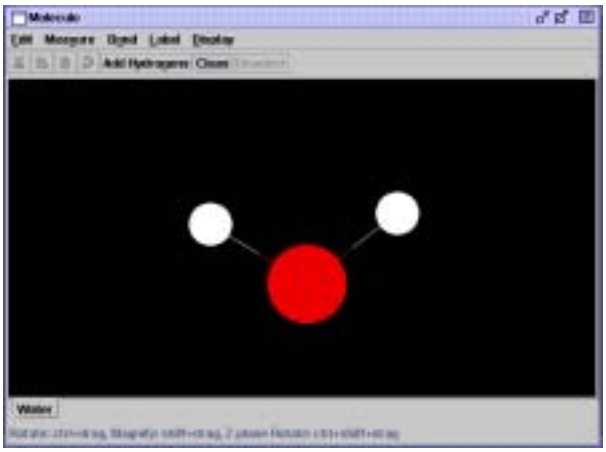
Rename the selected **Builder Panel**.

Example: Change the name 'Molecule 1' to 'Water'.

Procedure 1) Select **Rename Molecule 1** from the **Edit** menu in the **Builder Panel**.

Procedure 2) Change the name 'Molecule 1' to 'Water' in the **Rename Molecule** display. After clicking OK, this panel is renamed.





1)-d. Close…

Close the selected **Builder Panel**.

Example: Close the 'Water' **Builder Panel**.

Procedure 1) Select **Close Water** from the **Edit** menu in the **Builder Panel**.

Procedure 2) Close Molecule dialog will be appeared. OK for closing this file.

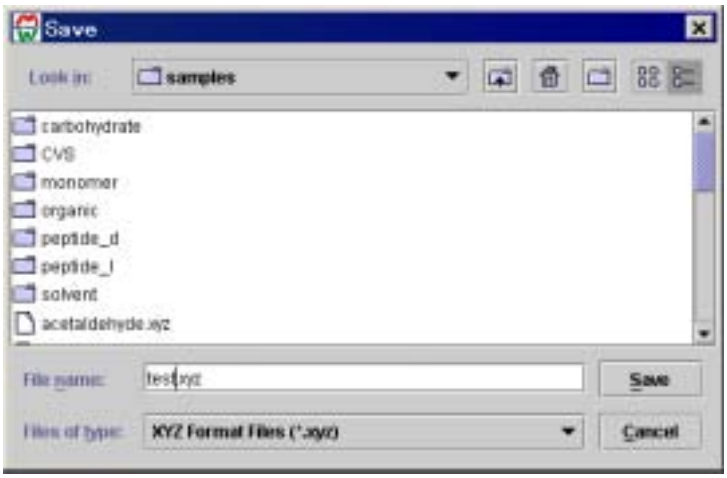
1)-e. Save As…

Save the molecular structure displaying in the **Builder Panel**.

Example: Save the geometry of acetaldehyde as test.xyz file

Procedure 1) Select **Save As…** from **Edit** menu in the **Builder Panel**.

Procedure 2) The browser for **Save** file will be appeared. After changing the file name 'acetaldehyde.xyz' to 'test.xyz', press Save.



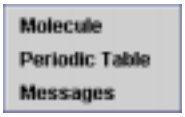
Procedure 3) If the same file name already exists there, following message dialog will

be displayed.

1)-f. Exit

Display the **Exit** dialog.

2) View



2)-a. Molecule

Display the **Molecule Window**. When the **Molecule Window** is already displayed, it comes to the front of the display.

2)-b. Periodic Table

Display the **Periodic Table Window**. When the **Periodic Table Window** is already displayed, it comes to the front of the display.

2)-c. Messages

Display the **Messages Window**. When the **Messages Window** is already displayed, it comes to the front of the display.

3) MO

3)-a. Interface

Display the **Simplified Setting Window** for creating input files for Q-Chem, Gaussian, GAMESS and MOPAC.

3)-b. Calc

Display the **CNDO/2 Window** for CNDO/2 calculation.

4) Properties

4)-a. Estimation

Display the **Estimation Window**.

5) Window

5)-a. Already existed window(s)

Checked window brings to the front of the display.

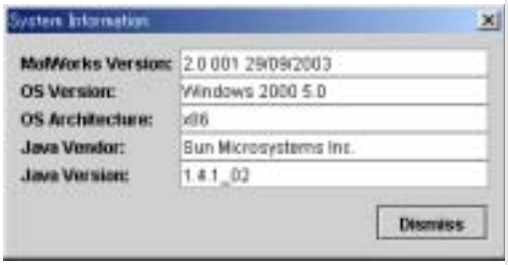
6) Help

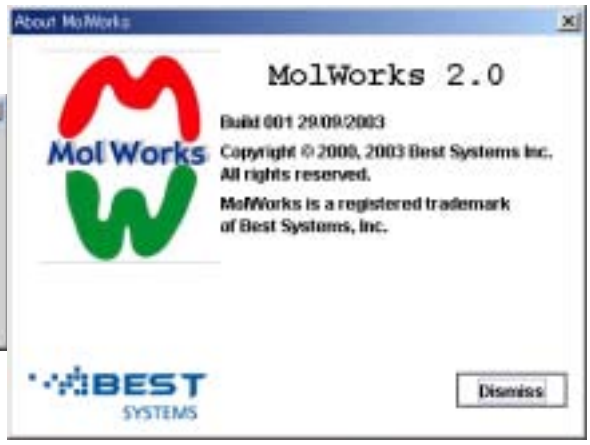
6)-a. System Information

MolWorks displays the **System Information** dialog box.

6)-b. About MolWorks

The **About MolWorks** dialog box is displayed.





II. Main Window

For the following windows: **Molecule Window**, **Periodic Table Window**, **Simplified Setting Window**, **MO Window**, **MO Setup Window**, **CNDO/2 Window**, **Estimation Window**, **Pure Properties Window**, **Properties Graph Window**, **Functional Groups Window**, **PVT Window** and **Messages Window** are displayed with in **Main Window**.

To minimize the window, click the button. The minimized window will be displayed at the bottom of the **Main Window**.

While the button is shown, you can change the size of the window. To maximize the window, click the button. To close the window, click the button.

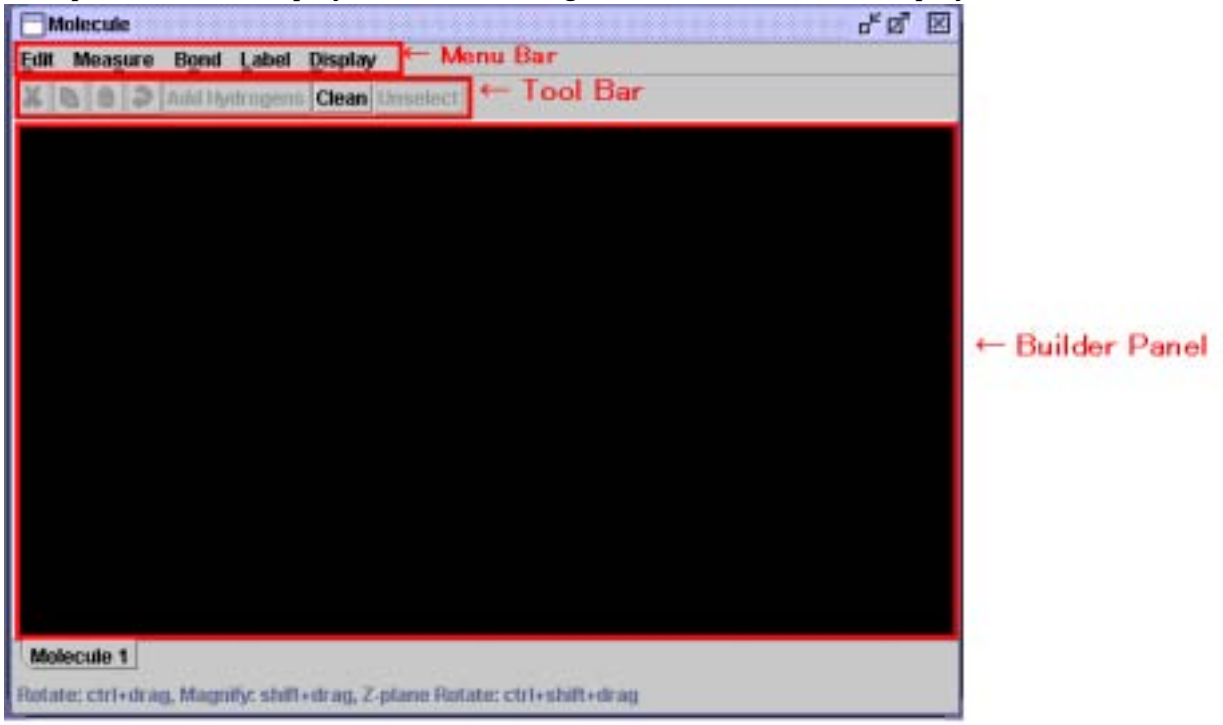
III. Status Bar

Choose the **Status Bar** from the **View** menu. The following status bar is displayed at the bottom of the **Main Window**:

① Messages are displayed here.
② The element type and the serial number of the atom are displayed here (e.g. C(1)).
③ Display the number of total atoms in the **Builder Panel** (e.g. Atom count: 8).
④ Mode is displayed here (Draw or Select).

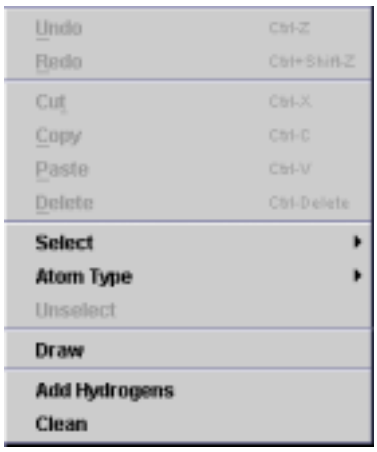
[5] Molecule Window

The **Molecule Window** consists of the **Menu Bar**, **Tool Bar**, and **Builder Panel**. In the **Builder Panel**, you can operate several molecules using tab panels. In the bottom of the window, the methods to manipulate for the displayed molecule using button and mouse are displayed.



I. Menu Bar

1) Edit



1)-a. Undo

Undo the previous editings.

1)-b. Redo

Redo the editings.

1)-c. Cut

Cut the selected atom(s).

1)-d. Copy

Not supported in Version 2.0.

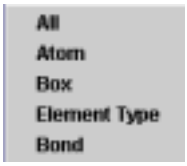
1)-e. Paste

Not supported in Version 2.0.

1)-f. Delete

Delete the selected atom(s).

1)-g. Select



1)-g-1: All

All atoms in the selected **Builder Panel** will be selected.

1)-g-2: Atom

The clicked atom(s) will be selected/unselected.

1)-g-3: Box

The white line box will be shown from the clicked point. All atom(s) in the white line box will be selected/ unselected.

1)-g-4: Element Type

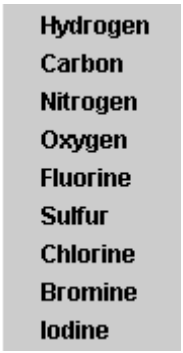
All atom(s) being a same element type with the clicked atom will be selected/ unselected.

1)-g-5: Bond

The clicked bond(s) will be selected/unselected.

1)-h. Atom Type

Choose the element type for drawing.



1)-i. UnSelect

When the selected atom(s) and/or bond(s) are existed, this command becomes active. When you choose this, all selected atom(s) and/or bond(s) will be unselected.

1)-j. Draw

Set the draw mode.

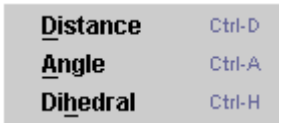
1)-k. Add Hydrogens

Adding the hydrogen atoms automatically considering the bond orders, distances, angles and dihedral angles.

1)-l. Clean

Execute a simple geometry optimization. If the energy is under 0.5 a.u. or the number of calculation cycles achieve 300, calculation is finished. If you open the new **Builder Panel** or select other **Builder Panel** during the calculation, optimization is stopped.

2) Measure



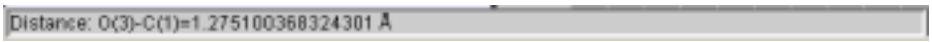
2)-a. Distance

Measure the distance between two selected atoms, and display the value in the **Status Bar** ①.

Example: Measurement of the C=O distance in 'acetaldehyde'

Procedure 1) Select **Distance** from the **Measure** menu. Then the following message appears in the **Status Bar** ①.

Procedure 2) Select two atoms in the **Builder Panel**. The distance is displayed in the **Status Bar** ①.



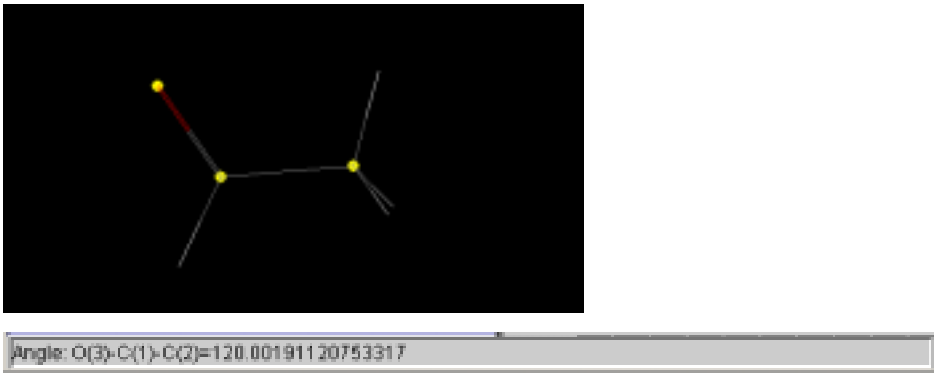
2)-b. Angle

Measure the angle between three selected atoms, and display the value in the **Status Bar** ①.

Example: Measurement of the O-C-C angle in 'acetaldehyde'

Procedure 1) Select **Angle** from the **Measure** menu. Then the following message appears in the **Status Bar** ①.

Procedure 2) Select three atoms in the **Builder Panel**. The angle is displayed in the **Status Bar** ①.



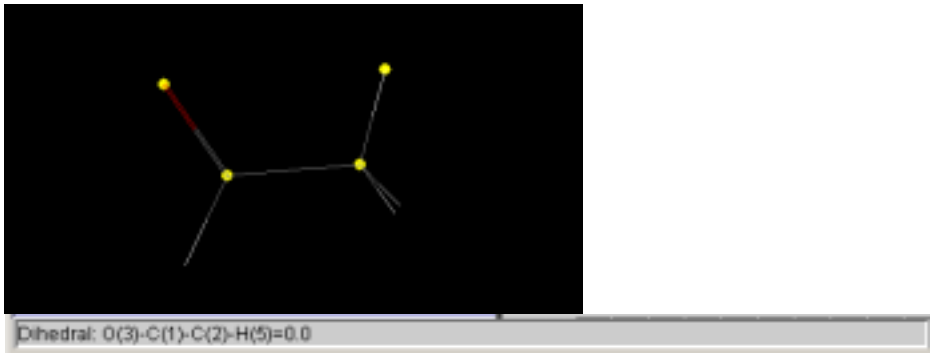
2)-c. Dihedral

Measure the angle between four selected atoms, and display the value in the **Status Bar** ①.

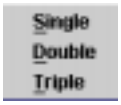
Example: Measurement of the O-C-C-O dihedral angle in 'acetaldehyde'

Procedure 1) Select **Dihedral** from the **Measure** menu. Then the following message appears in the **Status Bar** ①.

Procedure 2) Select four atoms in the **Builder Panel**. The dihedral angle is displayed in the **Status Bar** ①.



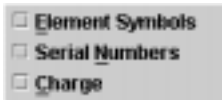
3) Bond



3)-a. Single · Double · Triple

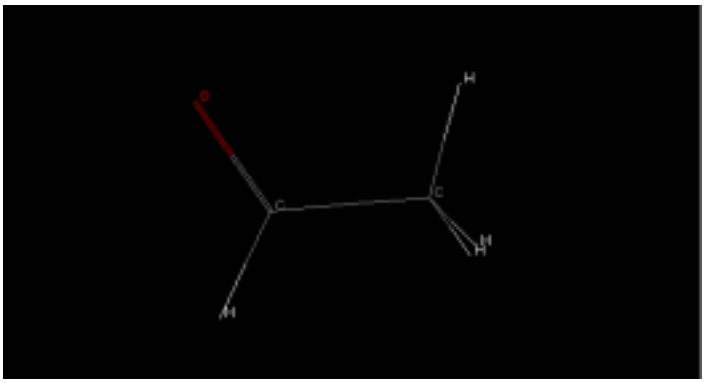
Change bond order of the selected bond to single, double, or triple.

4) Label



4)-a. Element Symbols

Display the element of each atom.



4)-b. Serial Numbers

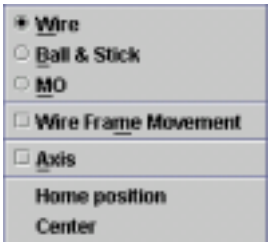
Display the serial number of each atom.

4)-c. Charge

Display the partial atomic charge of each atom after the results have been obtained from the CNDO/2 calculation.

※ **Element Symbols**, **Serial Numbers**, and **Charge** can be displayed simultaneously.

5) Display



5)-a. Wire

Display the molecule as a wire frame style.

5)-b. Ball & Stick

Display the molecule as a ball and stick style.

5)-c. MO

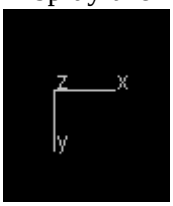
Display the molecular orbital, if the CNDO/2 calculation has already finished.

5)-d. Wire Frame Movement

Translation, rotation, and zoom of the molecule will be performed using the wire frame style (although the molecule is displayed in ball & stick style).

5)-e. Axis

Display the XYZ axes on upper left corner of the **Builder Panel**.



5)-f. Home position

Change the molecular direction to the one of the axes above, and move the center of mass of the molecule to the center of the **Builder Panel**.

5)-g. Center

Move the center of mass of the molecule to the center of the **Builder Panel**.

II. Tool Bar

Cut button. This button becomes active when one or more atoms are selected on the **Builder Panel**. The selected atoms are deleted when this button is pressed.

Copy button. Not supported in Version 2.0.

Paste button. Not supported in Version 2.0.

Undo button. Undo the previous editings.

Redo button. Redo the editings.

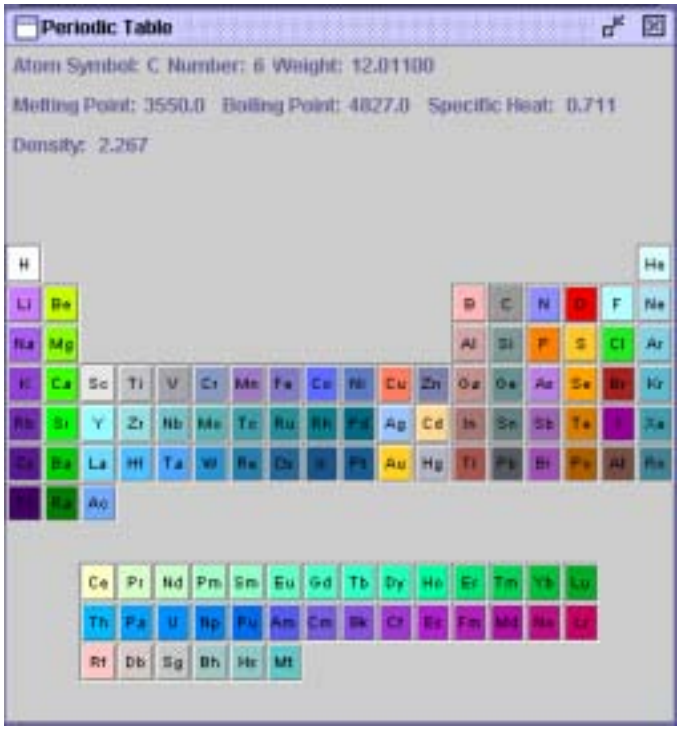
Add Hydrogens **Add Hydrogen** button. Adding the hydrogen atoms automatically considering the bond orders, distances, angles and dihedral angles.

Clean **Clean** button. Execute a simple geometry optimization.

[6] Periodic Table Window

In draw mode, element types can be selected by clicking the appropriate button. Also, clicking on the required element can change selected atoms in the **Builder Panel**. The background color of each element is adopted in the **Builder Panel**.

Also atomic number, mass of element (IUPAC), melting point, boiling point, specific heat and density are displayed at the top of the window.



[7] Simplified Setting Window

The **Simplified Setting Window** is the basic window to create the input files for Q-Chem, Gaussian, GAMESS and MOPAC. When you want to set any parameters, please click Advanced... . Then the **MO Window** will be displayed.

I. Selecting the Q-Chem button.

1) Save Input File

Save the Q-Chem input file for geometry optimization by RHF/STO-3G.

Example：H_2O

```
$comment
H2O
$end

$rem
JOBTYPE         SP
EXCHANGE        HF
BASIS           STO-3G
$end

$molecule
0 1
O   4.4300385   -1.6507636   -0.6619955
H   3.4728384   -1.6507636   -0.6619955
H   4.669702    -1.6507636   -1.5887065
$end
```

II. Selecting the Gaussian button

1) Save Input File

Save the Gaussian input file for geometry optimization by RHF/STO-3G.

Example：H_2O

```
#P   RHF/STO-3G   OPT

- Comment line -    H2O

01
O   0.0   0.0   0.0
H   0.96   0.0   0.0
H   -0.282   0.918   0.0
```

III. Selecting the GAMESS button

1) Save Input File

Save the GAMESS input file for geometry optimization by RHF/STO-3G.

Example：H_2O

```
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE COORD=CART ICHARG=0 MULT=1 $END
$BASIS GBASIS=STO NGAUSS=3 $END
$GUESS GUESS=HUCKEL $END
$DATA
- Comment line -     H2O
Cn 1

O   8   0.0    0.0    0.0
H   1   0.96   0.0    0.0
H   1   -0.282  0.918  0.0
$END
```

IV. Selecting the MOPAC button

1) Save Input File

Save the MOPAC input file for geometry optimization by PM3.

Example：H_2O

```
PM3 XYZ PRECISE
- Comment line -     H2O
- Comment line -
O   0.0     1 0.0     1 0.0 1
H   0.96    1 0.0     1 0.0 1
H   -0.282    1 0.918    1 0.0 1
```

V. Q-Chem・Gaussian・GAMESS・MOPAC

After clicking Advanced..., the **MO Window** is displayed.

[8] MO Window

The **MO Window** consists of four tabs concerned the four programs (Q-Chem, Gaussian, GAMESS, and MOPAC).

I. Q-Chem

Make input data for Q-Chem.

1) Calc. Type

Select the calculation type.

Single Point・Optimize・Frequencies・Transition Structure・Using data on right（other calculation type written in the text field is adopted）

2) Calc. Level

Select the calculation type.

RHF：Restricted Hartree-Fock
UHF：Unrestricted Hartree-Fock
ROHF：Restricted open shell Hartree-Fock
MP2：2nd order Moller-Plesset perturbation
CCD：Coupled Cluster with Doubles
CCSD：Coupled Cluster with Singles and Doubles
QCISD：Quadratic Configuration Interaction
OD：Optimized Orbital Coupled Cluster Doubles
BLYP：Becke exchange + LYP correlation
B3LYP：Becke's Three Parameter Hybrid Method Using the LYP Correlation
B3PW91：Becke's Three Parameter Hybrid Method Using the PW91 Correlation
EDF1：Empirical Density Functional 1
Using data on right：(other calculation type written in the text field is adopted)

3) Basis Set

Select the basis set.

STO-3G・3-21G・4-31G・6-31G・6-311G・Using data on right (other basis set written in the text field is adopted)

4) Polarization/Diffuse

Select the type of polarization and/or diffuse function.

Not used (Not including both polarization and diffuse.)**・*・**・+・++・* and +・** and +・** and ++**

5) Geometry

Specify the geometry type.

Cartesian : Set up the selected molecular geometry using the XYZ format automatically.

Modify : **Geometry Frame** is displayed. If **Save** button is pushed after changing structure data within the **Geometry Frame**, the changed structure save to the file.

6) Charge

Set the net charge of molecule.

7) Spin

Set the spin multiplicity of molecule.

8) Additional Keyword

Display the **Additional Keyword Frame**. Input keywords, and push the **Save** button when you want to add other optional keywords.

II. Gaussian

Make input data for Gaussian. The function to convert input data (Input Data Convert section) and to submit a Gaussian job (Run Gaussian Job section) can be used.

1) Output Level

Control the volume of output file.

#(normal) · **terse** · **detail**

2) Calc. Type

Select the calculation type.

Single Point · **Optimize** · **Freq** · **Optimize + Freq** · **Using data on right** (other calculation type written in the text field is adopted)

3) Calc. Level

Select the calculation level.

RHF : Restricted Hartree-Fock

UHF : Unrestricted Hartree-Fock

ROHF : Restricted open shell Hartree-Fock

CCD : Coupled Cluster with Doubles

CCSD : Coupled Cluster with Singles and Doubles

QCISD : Quadratic Configuration Interaction

MP2 : 2nd order Moller-Plesset perturbation

BLYP : Becke exchange + LYP correlation

B3LYP : Becke's Three Parameter Hybrid Method Using the LYP Correlation

Using data on right (other calculation level written in the text field is adopted)

4) Basis Set

Select the basis set.

STO-3G · 3-21G · 4-31G · 6-31G · 6-311G · Using data on right (other basis set written in the text field is adopted)

5) Polarization/Diffuse

Select the type of polarization and/or diffuse function.

Not used (Not including both polarization and diffuse.) **· * · ** · + · ++ · * and + · ** and + · ** and ++**

6) Geometry

Specify the geometry type.

XYZ.auto : Set up the selected molecular geometry using the XYZ format automatically.

Modify : **Geometry Frame** is displayed. If **Save** button is pushed after changing structure data within the **Geometry Frame**, the changed structure save to the file.

7) Charge

Set the net charge of molecule.

8) Spin

Set the spin multiplicity of molecule.

9) Additional Keyword

Display the **Additional Keyword Frame**. Input keywords, and push the **Save** button when you want to add other optional keywords.

10) Input Data Conversion

Convert the input data for Gaussian into the input data for Q-Chem, and save the converted data to file as a Q-Chem format. If **Save** button in **Input Data Conversion** section is pushed after editing input data on the Gaussian tab, the conversion is carried out.

11) Run Gaussian Job

If **Run** button in Run Gaussian Job section is pushed, the Gaussian program is executed. At first, input data edited in the Gaussian tab is saved at a file, then the Gaussian job is submitted. (To use this function, the Gaussian need to be installed locally. And some setup is required at **Setup Window.**

III. GAMESS

Make input data for GAMESS (The General Atomic and Molecular Electronic Structure System).

1) Calc. Type

Select the calculation type.

Single Point・**Gradient**・**Optimize**・**Frequencies**・**Using data on right** (other calculation type written in the text field is adopted)

2) Optimize Cycle

Specify the maximum number of iteration for geometry optimization. This button becomes active only in the case that **Optimize** is selected in **Calc. Type**.

3) Optimize Precision

Specify the precision of geometry optimization. This button becomes active only in the case that **Optimize** is selected in **Calc. Type**.

4) Calc. Level

Select the calculation level.

RHF : Restricted Hartree-Fock

UHF : Unrestricted Hartree-Fock

ROHF : Restricted open shell Hartree-Fock

Using data on right (other calculation level written in the text field is adopted)

5) Geometry

Specify the geometry type.

XYZ.auto : Set up the selected molecular geometry using the XYZ format automatically.

Modify : **Geometry Frame** is displayed. If **Save** button is pushed after changing structure data within **Geometry Frame**, the changed structure save to the file.

6) Basis Set

Select the basis set.

STO-3G・**3-21G**・**4-31G**・**6-31G**・**6-311G**・**Using data on right** (other basis set written in the text field is adopted)

7) Polarization

Select the type of polarization function.

not used・**p (for H-He)**・**d**・**f (for Li-Cl)**・**p,d**・**d,f**・**p,d,f**

8) Diffuse

Select the type of diffuse function.

not used・**s(for hydrogen)**・**s,p(for heavy atoms)**・**s,p(for all atoms)**

9) Time Limit

Set the maximum time of calculation **(minute)**.

10) Memory

Set the maximum memory used for calculation.

11) Charge

Set the net charge of molecule.

12) Spin

Set the spin multiplicity of molecule.

13) 

Display the **Additional Keyword Frame**. Input keywords, and click the **Save** button if you want to add other optional keywords.

IV. MOPAC

Make input data for MOPAC6 and MOPAC7.

1) Calc. Method

PM3 · AM1 · MNDO · MINDO/3

2) Calc. Type

Optimize · Frequencies · Thermo Data · Keyword (other calculation type written in the text field in the **Calc. Type Parameters** is adopted)

3) Geometry

Specify the geometry type.

XYZ.auto : Set up the selected molecular geometry using the XYZ format automatically.

Modify : **Geometry Frame** is displayed. If **Save** button is pushed after changing structure data within the **Geometry Frame**, the changed structure save to the file.

4) Calc. Type Parameters

4)-a. Optimize Algorithm

Select the algorithm for geometry optimization. This button becomes active only in the case that **Optimize** is selected in **Calc. Type**.

EF (Eigenvector Following) · BFGS

4)-b. Thermo Data

4)-b-1: Initial Temp.

Specify the initial temperature. This field becomes active only in the case that **Thermo Data** is selected in **Calc. Type**.

4)-b-2: Final Temp.

Specify the final temperature. This field becomes active only in the case that **Thermo Data** is selected in **Calc. Type**.

4)-b-3: Step Number

Specify the step size of temperature. This field becomes active only in the case that **Thermo Data** is selected in **Calc. Type**.

4)-b-4: Symmetric Number

Specify the symmetric number of geometry. This field becomes active only in the case that **Thermo Data** is selected in **Calc. Type**.

Point group symmetry	Symmetric Number	Point group symmetry	Symmetric Number	Point group symmetry	Symmetric Number
C_1,C_i, C_s	1	D_2, D_{2d}, D_{2h}	4	C_v	1
C_2, C_{2v}, C_{2h}	2	D_3, D_{3d}, D_{3h},	6	D_h	2
C_3, C_{3v}, C_{3h}	3	D_4, D_{4d}, D_{4h}	8	T, T_d	12
C_4, C_{4v}, C_{4h}	4	D_6, D_{6d}, D_{6h}	12	O_h	24
C_6, C_{6v}, C_{6h}	6	S_6	3		

4)-c. Interatomic Distance Check

Write the keyword **GEO-OK (ON)** or not **(OFF)**. **GEO-OK** override the job termination, which is due to that two atoms are within 0.8 Å of each other.

4)-d. Orbital output

Specify which the enable or disable to display the information of molecular orbital.

4)-e. Time Limit

Set the maximum time length of calculation (by the selected unit).

4)-f. Charge

Set the net charge of molecule.

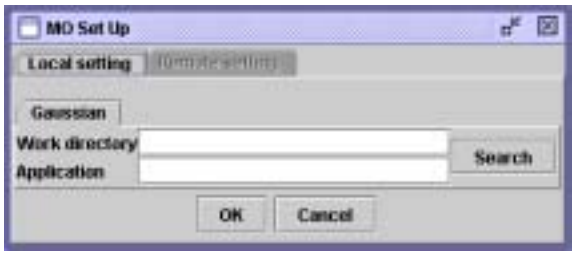
4)-g. Spin

Set the spin multiplicity of molecule.

4)-h. 

Display the **Additional Keyword Frame**. Input keywords, and push the **Save** button when you want to add other optional keywords.

[9] Setup Window



1) Work Directory

Set a default directory for saving a Gaussian input data file

2) Application

Set the executable file of Gaussian. (In the case of Gaussian98, it is set to g98 (Linux) or g98.exe (Windows))

The above two items are set using the **Search** button. If **OK** button is pushed, the setup

becomes effective.

3) Other setup

In addition to a setup on the Setup Window, the following setup is necessary for submitting Gaussian jobs. (The method for setting up in the case of using Gaussian98 is shown as an example. Please refer to the Gaussian manual for details)

3)-a. Linux

Before starting the MolWorks, a setup of an environment variable, g98root, and execution of a script is required. In the following examples, it is assumed that the Gaussian is installed at /opt/g98.

In the case of C shell
setenv g98root /opt
source $g98root/g98/bsd/g98.login

In the case of BA shell
export g98root=/opt
source $g98root/g98/bsd/g98.profile

If the above-mentioned procedures are described to .cshrc file (C shell) or .bashrc file (BA shell), the setup is available whenever the shell is started. This can be used when executing MolWorks from a command line.

If the above-mentioned procedures are described to .login file (C shell) or .bash_profile file (BA shell), the setup is available whenever a user logs in. This can be used when executing MolWorks by the double click of a mouse.

3)-b. Windows

Before starting the MolWorks, it is necessary to add the directory where the Gaussian is installed (ex. C:¥G98W) to an environment variable, PATH.

[10] CNDO / 2 Window

Execute the CNDO/2 calculation.(Maximum # of atoms: 100, Maximum # of orbitals: 300)

I. Input Parameters

1) SCF convergency

This parameter decides the precision of SCF calculation (thresh hold of the difference of molecular orbital energies). Default value is set to 0.000001.

2) Max Cycles

This parameter decides the maximum number of iteration of SCF calculation. Default value is set to 100.

3) Charge

Set the net charge of molecule.

4) Spin

Set the spin multiplicity of molecule (only the singlet state is supported in version 2.0).

II. Results

1) Number of Cycle

Display the actual iteration number of SCF calculation.

2) Energy Difference (a.u.)

Display the maximum value of the difference of molecular total energies in the iteration.

3) Energy (a.u.)

Display the total energy of the molecule.

III. Dipole Results

1) Dipole (debye)

Display the absolute value of dipole moment.

2) X (debye),Y (debye),Z (debye)

Display the component of dipole moment along X, Y, and Z direction.

IV. Calculate

Execute the CNDO/2 calculation.

V. MOs

Display the **MO Control Window** and the shape of highest occupied molecular orbital (HOMO) in the **Builder Panel**. This button becomes active only in the case that the CNDO/2 calculation

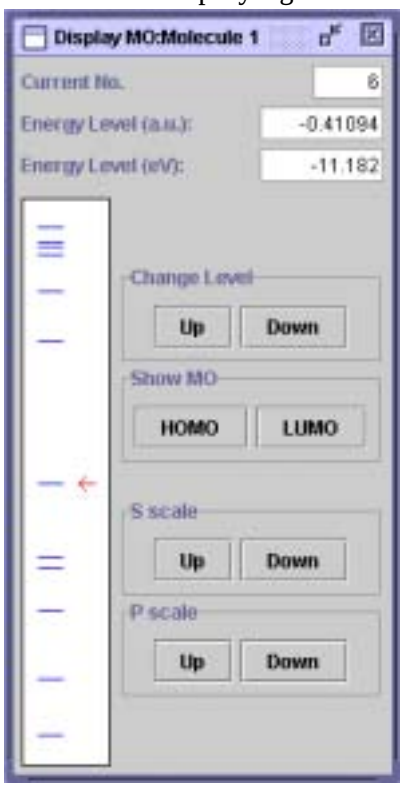
is converged.

VI. 

Calculate and display the absolute value of dipole moment, and its component along X, Y, and Z-axes. This button becomes active only in the case that the CNDO/2 calculation is converged.

[11] Display MO Window

Control the displaying molecular orbital resulted by CNDO/2 calculation.



I. Current Energy Level

Display the energy of selected orbital (indicated by red arrow).

II. Change Level

Up or down the level of molecular orbital displayed within the **Builder Panel**.

III. S Scale

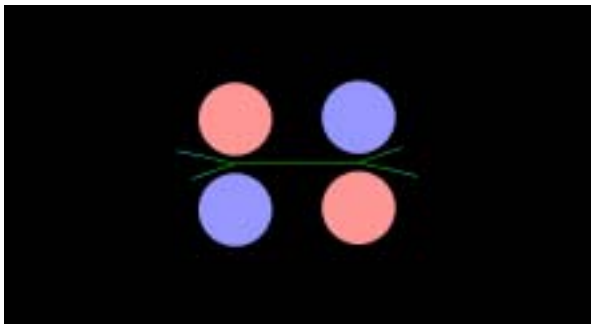
Multiply or reduce of S orbital component of molecular orbital displayed within the **Builder Panel**.

IV. P Scale

Multiply or reduce of P orbital component of molecular orbital displayed within the **Builder Panel**.

V. Show MO

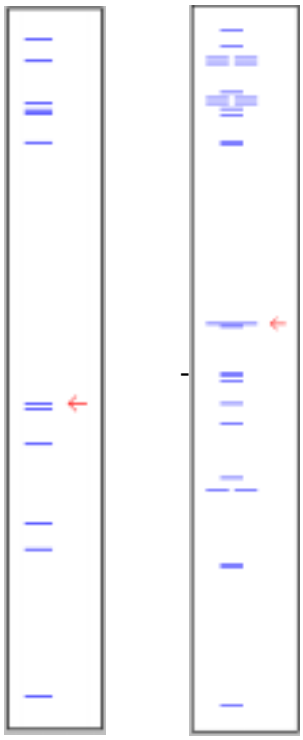
Set the molecular orbital displayed within the **Builder Panel** to HOMO[1)] or LUMO[2)].
Example: The LUMO of ethylene.



[1] Highest Occupied Molecular Orbital. [2] Lowest Unoccupied Molecular Orbital.

VI. MO Level

All of the molecular orbitals are displayed. The red arrow points the level of selected orbital. If the orbital set that the difference of orbital energies is below 0.0001 hartree is existed (i.e., degenerated orbitals are existed), it displays as right-hand below.



[12] Estimation Window

I. Pure Properties

1) Molecule

All molecules displayed in the **Molecule Window** are listed in the pull down menu. When certain molecule is selected in the pull down menu, this molecule is displayed in the **Builder Panel** automatically. And when certain molecule is selected in the **Builder Panel**, this molecule is displayed in this menu automatically.

2) Parameter

Select the parameter for estimation.

2)-a. Joback

Joback, K. G., "S.M. thesis in chemical engineering", Massachusetts Institute of Technology, Cambridge, Massachusetts, **1984**.

2)-b. Modified Joback

Use Joback parameters determined by us with some modification.

3) Calculate

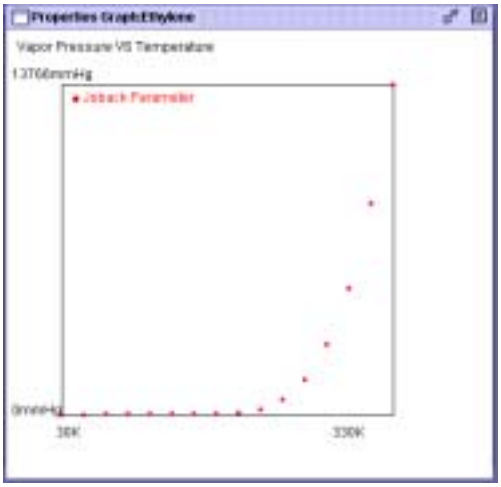
Estimate the pure properties of molecule using selected parameter. And display the **Pure Properties Window** and the **Functional Groups Window** (the groups and the number of each groups using in the calculation are displayed within this window).

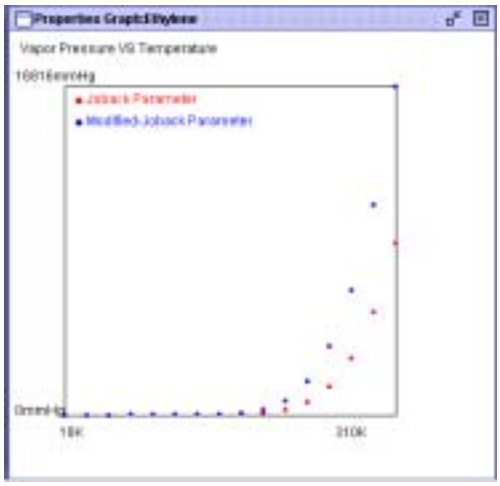
4) Graph

Select the property for plotting the graph. Only the vapor pressure is supported in version 2.0.

4)-a. Show

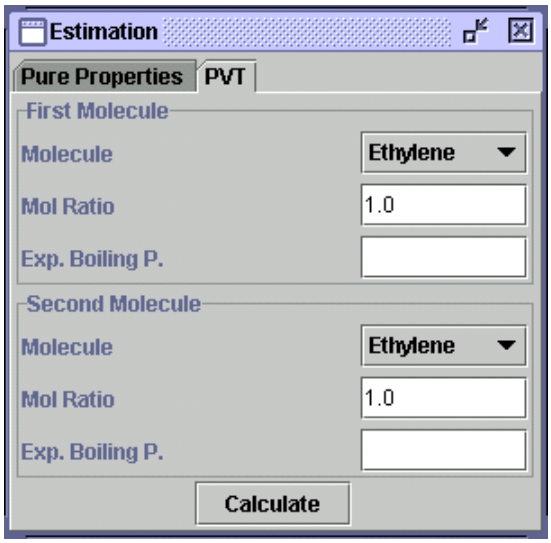
Display the graph of selected properties vs. temperature.

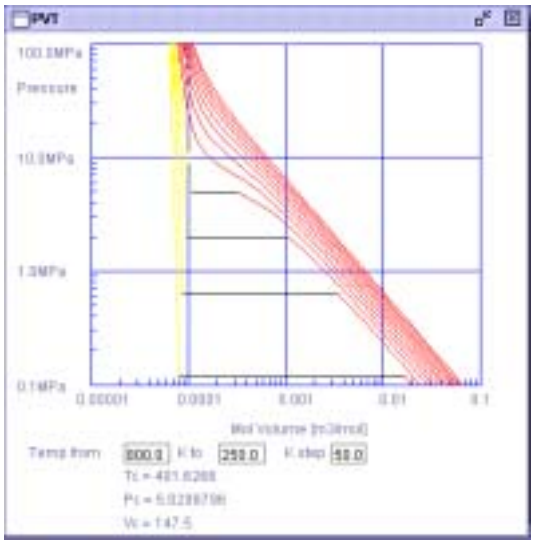




II. PVT

Draw the **PVT** (Pressure – Volume – Temperature) **graph**.





1) First Molecule

Specify the first molecule and condition.

1)-a. Molecule

Select molecule in the **Builder Panel**.

1)-b. Mol Ratio

Set the ratio of mixture.

1)-c. Exp. Boiling P.

Set the experimental boiling point if you already know. If you set it, the estimation is more accurate. If you don't set this, estimated boiling point from Joback parameter is used.

2) Second Molecule

Specify the second molecule and condition.

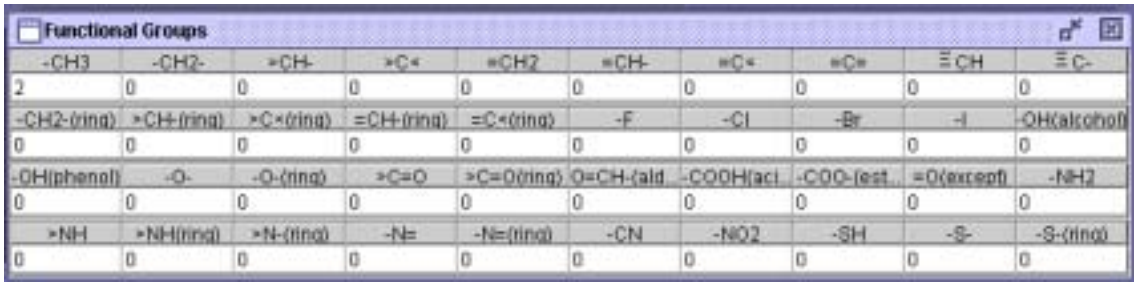
The descriptions of the settings for second molecule are same as above.

3) Calculate

Estimate properties and draw **PVT graph** using condition in **First** and **Second Molecule**.

[13] Functional Groups Window

This window displays the groups and the number of each group used for properties estimation.



[14] Messages Window

Display the messages of **MolWorks**.

[15] How to use mouse

Rotate: ctrl+drag, Magnify: shift+drag, Z-plane Rotate: ctrl+shift+drag

I. Rotation

When you move a cursor to right or left on the **Builder Panel** with holding on the control button, the molecule will be rotated by Y-axis. When you move a cursor to up or down on the **Builder Panel** holding on the control button, the molecule rotate by X-axis.

II. Rotation (Z axis: perpendicular to the window)

When you move a cursor to right or left on the **Builder Panel** with holding on the control button and the shift button, the molecule rotates on Z-axis.

III. Magnification and Reduction

When you move a cursor to the right on the **Builder Panel** holding on the shift button, the molecule is magnified. When you move a cursor to left on the **Builder Panel** holding on the shift button, the molecule is reduced.

[16] About dealing molecule(s)

I. Max atoms

1000 atoms

II. Move atom(s)

1) Moving all atoms

You should click the left button of mouse and drag the pointer to the place where you want.

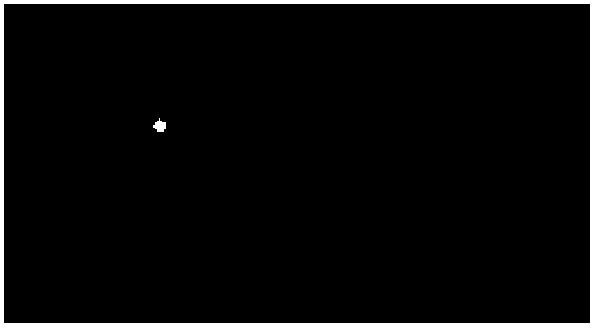
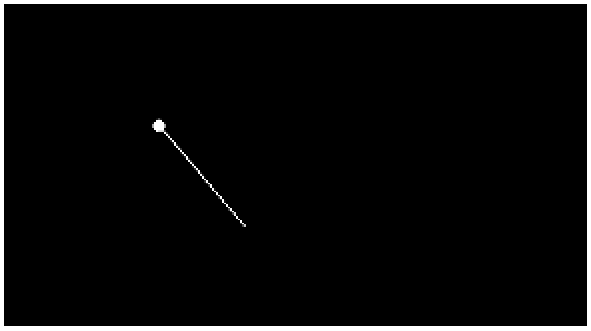
2) Moving the selected atom

You should click the right button of mouse and drag the pointer to the place you want.

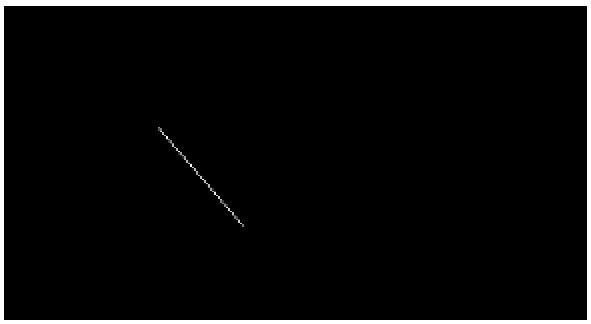
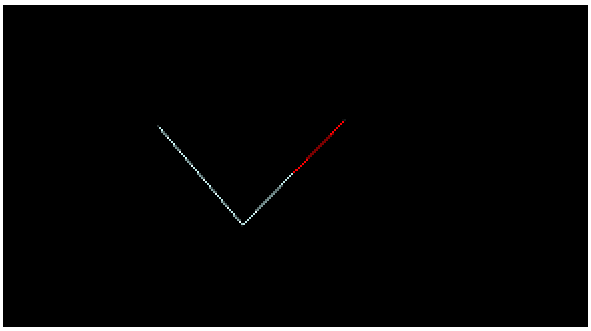
III. Building the molecule

Example: building ethanol

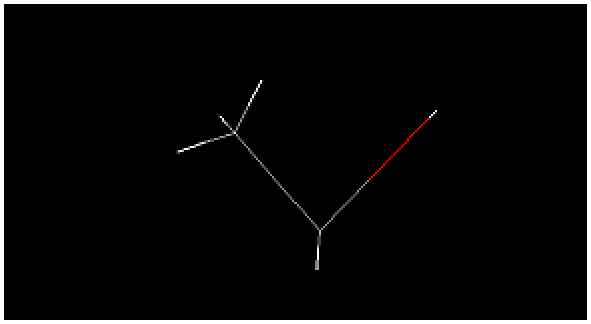
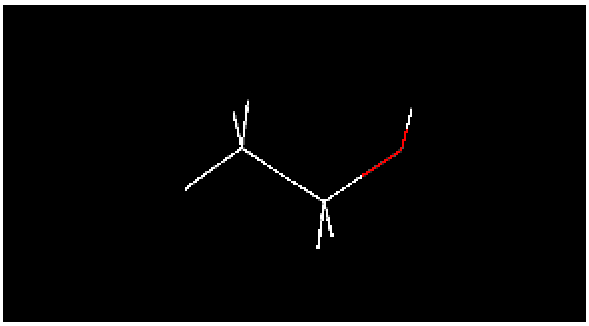
Procedure 1) If you select **New** from **File** of the menu bar, new molecule panel is shown. When you click on the **Builder Panel**, one carbon atom is displayed (Carbon is the default atom).
Procedure 2) When you move mouse pointer, the white line is drawn from the first carbon.

Procedure 3) If you click the point you want to place the second carbon, C-C bond is drawn.
Procedure 4) If you want to change the selected atom from carbon to oxygen, you should click **O** on the **Periodic Table Window** or selecting **Edit** -> **Atom Type** -> **Oxygen** from menu bar of the **Molecule Window**.
Procedure 5) When you click the second carbon and move a pointer, the white line appears from the second carbon. When you click the point you want to place the oxygen, the C-C-O is drawn.

Procedure 6) Hydrogen(s) are added by clicking Add Hydrogens from the **Tool Bar** or selecting **Edit** -> **Add Hydrogens** from menu bar of the **Molecule Window**.
Procedure 7) The molecule cleaned up by clicking Clean from the **Tool Bar** or selecting **Edit** -> **Clean** from menu bar of **Molecule Window**.

[17] Supported file format

I. Import

XYZ Format Files(*.xyz)
Protein Data Bank File(*.pdb)
Q-Chem Input File(*.in, *.inp)
Q-Chem Output File(*.out, *.log, *.ref)
Gaussian Input File(*.com, *.inp)
Gaussian Output File(*.out, *.log)
GAMESS Input File(*.com, *.inp)
GAMESS Output File(*.out, *.log)
MOPAC Input File(*.dat)
MOPAC Output File(*.out)

II. Export

XYZ Format Files(*.xyz)

III. XYZ type

Comment **(First line)**
Atom type X coordinate Y coordinate Z coordinate **(After the second line)**

[18] Properties Estimation

I. Groups for estimation in this program

$-CH_3$(non-ring)	$-CH_2-$(ring)	−OH(phenol)	>NH(non-ring)
$>CH_2$(non-ring)	>CH−(ring)	−O−(non-ring)	>NH(ring)
>CH−(non-ring)	>C<(ring)	−O−(ring)	>N−(non-ring)
>C<(non-ring)	=CH−(ring)	>C=O(non-ring)	−N=(non-ring)
$=CH_2$(non-ring)	=C<(ring)	>C=O(ring)	−N=(ring)
=CH−(non-ring)	−F	O=CH−(aldehyde)	−CN
=C<(non-ring)	−Cl	−COOH(acid)	$-NH_2$
=C=(non-ring)	−Br	−COO−(ester)	−SH
≡CH(non-ring)	−I	=O(except as above)	−S−(non-ring)
≡C−(non-ring)	−OH(alcohol)	$-NH_2$	−S−(ring)

II. Properties

1) Joback

Joback Method Boiling Point (K) / (℃)
Joback Method Freezing Point (K) / (℃)
Joback Method Critical Temperature Tc (K) / (℃)
Joback Method Critical Pressure Pc (bar) / (atm)
Joback Method Critical Volume Vc (cm^3/mol)
Edmister Method omega (From Joback Parameter Acentric Factor)
Lee-Kesier Method omega (From Joback Parameter Acentric Factor)
Critical Compressibility factor Zc
Yen-Woods Method Density (g/cm^3)
Reidel Method Vapor Pressure (mmHg)
Vetre Method Heat of Vaporization (at boiling point) (cal/mol)
L-J Collision Diameter for Chemkin program(Å)
L-J Well Depth for Chemkin program(J/mol)

2) Modified Joback

Modified Joback Boiling Point (K) / (℃)
Modified Joback Critical Temperature (K) / (℃)
Modified Joback Critical Pressure (bar) / (atm)
Modified Joback Critical Volume (cm^3/mol)
Edmister Method omega
Lee-Kesler Method omega
Critical Compressibility factor Zc
Density Estimation (at 298K) (g/cm^3)
Yen-Woods Density Estimation (g/cm^3)
Riedel Vapor Pressure (at 298K) (mmHg)
Vetre Method Heat of Vaporization. (at boiling point) (cal/mol)
Heat Capacity Estimation (at 298K) (cal/mol K)
Gibbs Energy (kcal/mol)
Heat of Formation (kcal/mol)
Thermal Conductivity (at 298K) (mW/mK) of Gas
Thermal Conductivity (at 298K) (mW/mK) of Liquid
Molecular Surface Estimation ($Å^2$)
Molecular Volume Estimation ($Å^3$)
Surface Tension Estimation (at 298K) (dyne)

[19] References

●CNDO/2
Pople, J. A., Beveridge, D. L., “Approximate Molecular Orbital Theory”, McGraw-Hill, New York, **1970**.

●Gaussian
http://www.gaussian.com/

●GAMESS
http://www.msg.ameslab.gov/GAMESS/GAMESS.html

●MOPAC
[1] Dewar, M.J.S., Thiel, W., *J. Am. Chem. Soc.*, **1977**, *99*, 4899, 3907.
[2] Dewar, M.J.S., Zoebisch, E.G., Healy, E.F., Stewart, J..P., *J. Am. Chem. Soc.*, **1985**, *107*, 3902.,
[3] Dewar, M.J.S., Stroch, D.M., *J. Am. Chem. Soc.*, **1985**, *107*, 3898.
[4] Stewart, J.J.P., *J. Comput. Chem.*, **1989**, *10*, 209, 221.

●Q-Chem
http://www.q-chem.com/

●Joback
Joback, K. G., “S.M. thesis in chemical engineering”, Massachusetts Institute of Technology, Cambridge, Massachusetts, **1984**.

Please send the bug reports to following e-mail address.
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