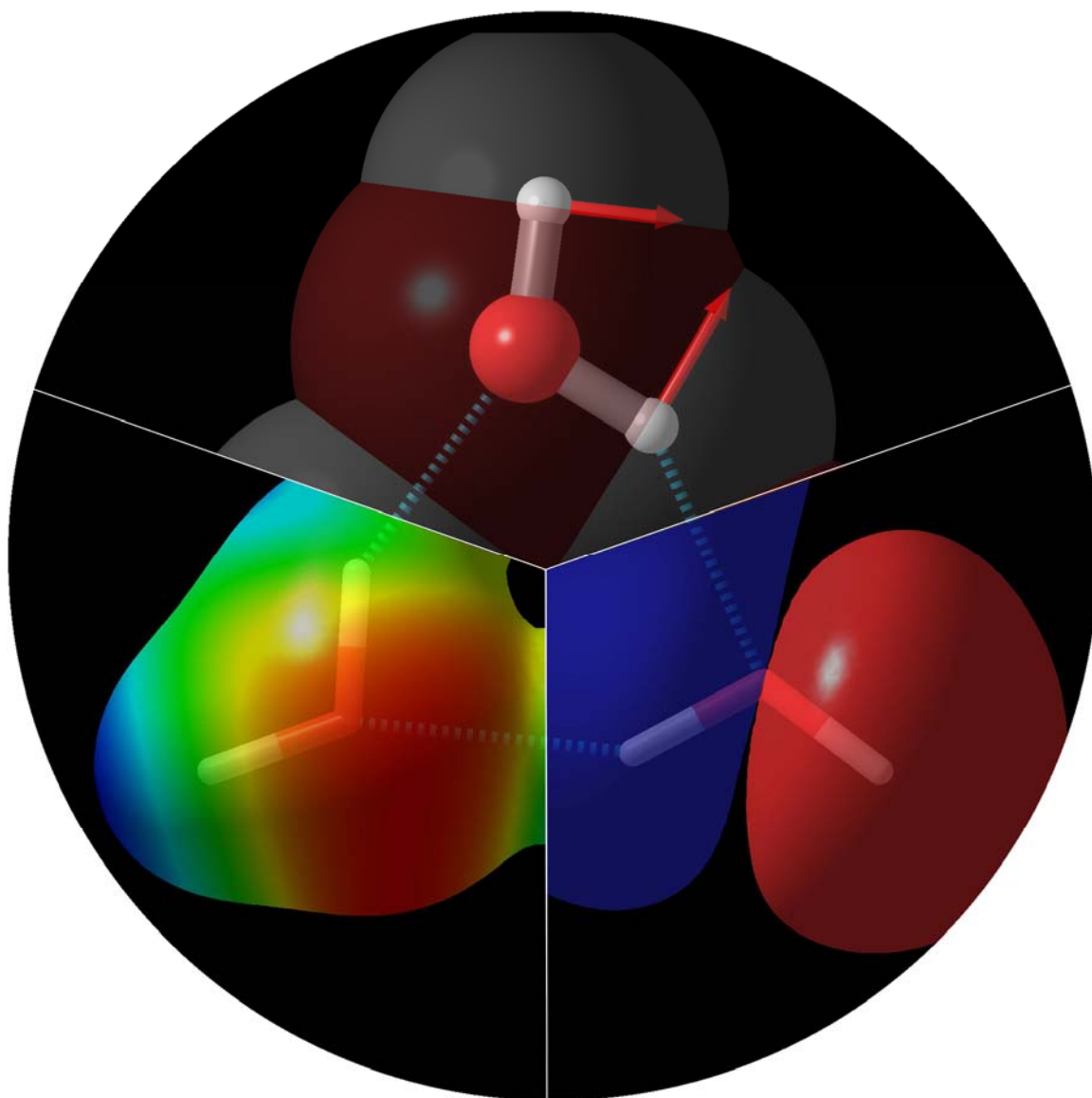


# Molecular Modeling and Simulation Kit



::MaSK::

Author: Yevgeniy Podolyan, Ph.D.



© 2006-2007 Computational Center for Molecular Structure and Interactions

# Table of Contents

1. Introduction.....	3
1.1 About MaSK.....	3
1.2 Using MaSK with GAMESS .....	4
1.3 Using MaSK with Gaussian®.....	5
2. Menus and Toolbars.....	5
2.1 Menus.....	5
2.2 Toolbars .....	9
3. Molecule Visualization and Manipulation.....	11
3.1 Opening and Saving a File.....	11
3.2 Changing Molecule's Visualization Mode.....	11
3.3 Showing Additional Information .....	11
3.4 Zooming In/Out .....	12
3.5 Measuring .....	12
3.6 Molecule Manipulation.....	12
4. Working with Output Files .....	13
4.1 Visualization of Optimization.....	13
4.2 Visualization of Molecular Properties .....	14
4.2.1 Dipole Moment .....	14
4.2.2 Mulliken and Lowdin Charges.....	14
4.2.3 Molecular Orbitals .....	15
4.2.4 Electron and Spin Densities .....	17
4.2.5 Molecular Electrostatic Potential.....	18
4.3 Visualization of Molecular Vibrations.....	19
4.4 Viewing Result Summaries.....	20
4.5 Exporting PES Scan Result (GAMESS).....	20
5. Converting Output to Input.....	20
6. Working with Input Files .....	21
6.1 Modifying Geometry .....	21
6.2 Adding Atoms.....	23
6.3 Adding Groups of Atoms.....	24
6.4 Setting GAMESS Input Options.....	25
6.5 Running GAMESS Calculations.....	27
7. Saving, Printing and Copying Images .....	28
8. Exporting Cartesian Coordinates .....	28
9. Customizing MaSK.....	29
9.1 General.....	29
9.2 Visualization .....	30
9.3 Atoms.....	31
9.4 Bonds .....	32

# 1. Introduction

## 1.1 About MaSK

Molecular Modeling and Simulation Kit (MaSK) is the software that is useful in the visualization of various molecular properties calculated by either GAMESS or Gaussian<sup>®</sup> computational chemistry programs. MaSK can also be used to create, modify and set options for the PC GAMESS input files. The user will also be able to run the PC GAMESS job and control its execution without leaving the MaSK interface.

Key features of MaSK include ability to:

General:

- Read 4 formats: GAMESS output, GAMESS input, Gaussian output, and Gaussian input
- Visualize molecules in 4 styles: balls and sticks, spheres, tubes, and wireframe
- Choose between orthographic and perspective view
- Show/hide hydrogen bonds, atom names and numbers
- Visualize coordinate axes
- Measure distances, angles, dihedral angles, and angles between planes (and monitor their changes during optimization)
- Save images as JPEG, GIF, BMP or PNG graphics files
- Copy image to the clipboard to paste in other application
- Modify input geometry as Z-matrix (including automatic and manual atom addition or automatic functional group addition) or Cartesian coordinates
- Set input options for GAMESS job and save as GAMESS Input file
- Submit GAMESS (PC GAMESS version) job from within the MaSK
- Check the status of a PC GAMESS calculation
- Terminate PC GAMESS calculation

Results:

- Visualize all steps of optimization as a movie or step-by-step
- Visualize all optimized points of the Intrinsic Reaction Coordinate (IRC) following
- Visualize calculated Mulliken (GAMESS and Gaussian) and Lowdin (GAMESS) charges
- Visualize vibrational modes as animation or as vectors
- View optimization energy graph (SCF-only energies for Gaussian output)
- Visualize dipole direction
- Visualize molecular orbitals with multiple options
- Visualize electron and spin densities
- Visualize molecular electrostatic potential plotted onto the electron density
- Show brief or extended summaries of the results
- Export Potential Energy Surface scan results from GAMESS calculations to CSV file format for use in spreadsheet applications

Customization:

- Change text size and color
- Change background color
- Choose maximum resolution of the saved images
- Choose to draw/hide metal-metal bonds
- Choose to draw/hide metal-nonmetal bonds
- Change the speed of rotation of the molecule, vibrations, and animation of optimization steps
- Change atomic parameters for any atom:
  - 1) Atomic radius
  - 2) Van der Waals radius
  - 3) Atom color
- Modify radius and color of covalent and hydrogen bonds as well as opacity of hydrogen bonds.

## 1.2 Using MaSK with GAMESS

GAMESS (The **G**eneral **A**tom and **M**olecular **E**lectronic **S**tructure **S**ystem) is a general *ab initio* quantum chemistry package. There are several different version of GAMESS developed by different groups of researchers (e.g GAMESS-US, GAMESS-UK, etc.). MaSK was specifically developed with the support for PC GAMESS.

PC GAMESS is a freely available *ab initio* and DFT computational chemistry program developed to offer high performance on Intel-compatible x86, AMD64, and EM64T processors. It was initially based on the free GAMESS-US program sources but extends its functionality in some important areas. The PC GAMESS project is maintained by the staff of the Laboratory of Chemical Cybernetics at Moscow State University (MSU). The project coordinator and leading developer is Dr. Alex A. Granovsky. PC GAMESS can be obtained free of charge after registration from <http://classic.chem.msu.su/gran/gamess>.

The versions of GAMESS other than PC GAMESS can be read in most cases. However, the functionality of MaSK can be limited when working with unsupported versions of GAMESS.

GAMESS has a large number of options that control the type of calculations, properties being calculated and the amount of data the user wants to see in the output. It is recommended that when searching for optimal geometry or saddle point users do not use values -1 or -2 for the key NPRT in the \$STATPT group in GAMESS input as this turns off the printing of molecular orbital coefficients needed for molecular orbital visualization in MaSK. If a user creates GAMESS input file in MaSK, this option is automatically left at its default value (0).

PC GAMESS input files can be created from within MaSK. User can select from many built-in options such as run type, level of theory, SCF type, etc. Since GAMESS supports a very large number of options, the MaSK includes only a subset of those options. If the desired option(s) is not available in the options section, user can add/modify such option(s) manually in the created input file.

If the PC GAMESS is installed on the computer, user can submit the calculations, check the status of calculations, and read the results without ever leaving MaSK.

## 1.3 Using MaSK with Gaussian®

Gaussian® is a commercial electronic structure program and is available from <http://www.gaussian.com>. Gaussian is used by chemists, chemical engineers, biochemists, physicists and others for research in established and emerging areas of chemical interest.

Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures.

The MaSK is able to read and visualize multiple calculated properties from the Gaussian output file. However, the molecular energies shown by MaSK (optimization graph and results summaries) are the SCF energies. If the level of theory of performed calculations is other than Hartree-Fock or Density Functional Theory, the user is instructed to manually inspect the output file to find the final energy or energies at each optimization step at the desired level of theory.

Only the molecule's geometry can be read from the Gaussian input file; all Gaussian directives are omitted when reading the file. If the input file contains several jobs (separated with --Link1-- directive, only the first one will be read). Even though reading Gaussian input file is supported, the input file cannot be saved. Therefore, if user needs to modify and save the molecule read from the Gaussian input file, it may be [converted to GAMESS input](#) or the modified geometry may be [exported in a form of Cartesian coordinates](#) into a text file.

It is recommended to use the following options in the Route (#) section of Gaussian input:

1. GFInput to print basis set
2. Pop=Full (or Pop=NaturalOrbitals) to print molecular orbital coefficients

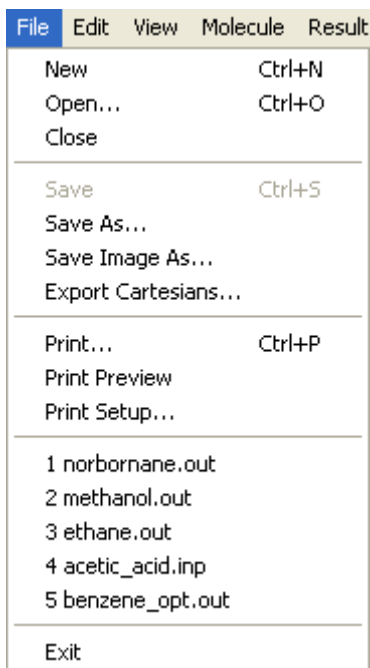
Without the above options, MaSK will not be able to visualize molecular orbitals, electron and spin densities, and molecular electrostatic potential.

## 2. Menus and Toolbars

### 2.1 Menus

The program has 7 popup menus in the top-level menu. They are

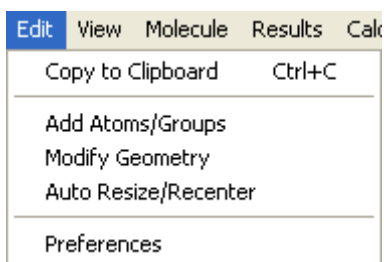
1. File
2. Edit
3. View
4. Molecule
5. Results
6. Calculate
7. Help



**Figure 2.1.** File menu.

The File menu (Fig. 2.1) has the following options:

1. New: Create a new GAMESS Input file
2. Open: Open existing supported file
3. Close: Close opened file
4. Save: Save opened GAMESS Input file (disabled for other file types)
5. Save As...: Save file as GAMESS Input
6. Save Image As...: Save screen image to JPEG, GIF, PNG, or BMP file
7. Export Cartesians...: [Export geometry as Cartesian coordinates](#) into a text file
8. Print...: Print screen image
9. Print Preview: Show a preview of the printed image on screen
10. Print Setup...: Set the printer and its options.
11. Five most recently opened files
12. Exit: close the program

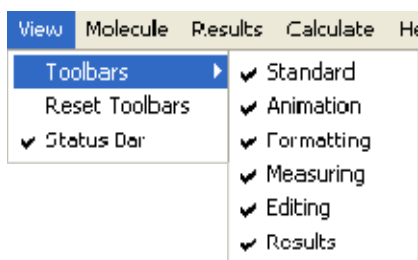


**Figure 2.2.** Edit menu.

The Edit menu (Fig. 2.2) has the following options:

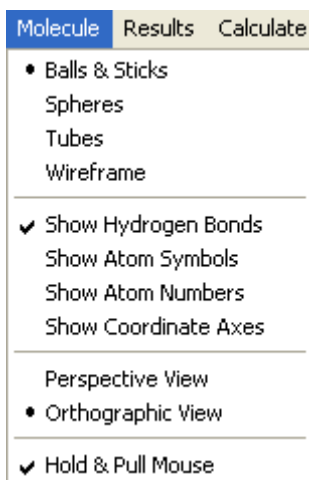
1. Copy to Clipboard: Copy the screen image to clipboard for later insertion in another application
2. Add Atoms/Groups: Open a dialog to add atoms or groups of atoms
3. Modify Geometry: Open a dialog to modify molecule's geometry in form of Z-Matrix or Cartesian coordinates

4. Auto Resize/Recenter: Resize the molecule to fit in the screen and recenter in the window (useful when adding atoms)
5. Preferences: Modify [program preferences](#)



**Figure 2.3:** View menu.

The View menu (Fig. 3) allows user to control which of the toolbars and whether the status bar are visible on the screen. By highlighting the Toolbars option, the new popup menu will show available toolbars and the checkmarks indicate which of them are currently visible. Selecting/deselecting a particular toolbar will show/hide this toolbar. Reset Toolbars option allows to reset the positions of all toolbars to their default locations and sets them all to visible state.



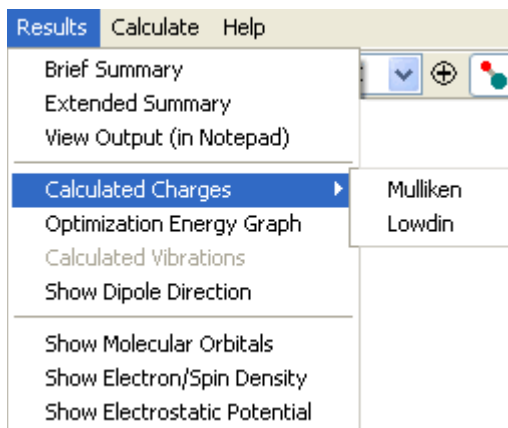
**Figure 2.4.** Molecule menu.

The Molecule menu (Fig. 2.4) contains options relevant to the way the molecule is drawn and manipulated on the screen. The following options are available:

1. Balls & Sticks: Show atoms as balls and bonds as sticks
2. Spheres: Show atoms as space-filling spheres
3. Tubes: Show molecules as tubes
4. Wireframe: Show molecules in form of thin wires  
*Note:* Only one option (1-4) can be selected at a time.
5. Show Hydrogen Bonds: Show/hide hydrogen bonds if present
6. Show Atom Symbols: Show/hide Atomic labels
7. Show Atom Numbers: Show/hide the number of each atom in the molecule
8. Show Coordinate Axes: Show/hide the coordinate axes (useful in building/modifying a molecule)

9. Perspective View: Show molecule in perspective projection (parts of the molecule that are closer to the viewer appear larger)
10. Orthographic View: Show molecule in orthographic projection (all parts of the molecule have the same size regardless of the distance from the viewer)
- Note: Only one option (Perspective or Orthographic) can be selected at a time.

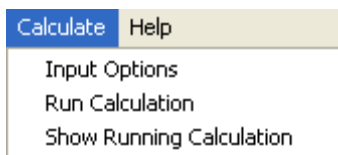
11. Hold & Pull Mouse: Use a sticky-type mouse pointer (selected) or a regular one (deselected). (See [Molecule manipulation](#) the for more details on this option)



**Figure 2.5.** Results menu.

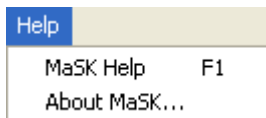
The Results menu (Fig. 2.5) contains the options to visualize various calculated properties. When a particular property has not been calculated or has not been properly read from the output file, the corresponding option in the Results menu will be disabled. All options in this menu are disabled for input files. Available options include:

1. Brief Summary: Show a summary of results such as type of calculation, level of theory, basis set, final energy, etc.
2. Extended Summary: Show more information from the output by adding energies at each step of geometry optimization, thermochemical data and calculated charges (if calculated) to the brief summary.
3. View Output (in Notepad): Open the output file in the Notepad text editor
4. Calculated Charges: Choose to show/hide Mulliken or Lowdin calculated charges on atoms
5. Optimization Energy Graph: Show the graph with relative energies at each step of geometry optimization
6. Calculated Vibrations: Show a dialog controlling the visualization of calculated molecular vibrations
7. Show Dipole Direction: represents the direction of the calculated dipole moment in the molecule (absent if 0)
8. Show Molecular Orbitals: Open a dialog to control the visualization and calculation of molecular orbitals
9. Show Electron/Spin Density: Open a dialog to control the visualization and calculation of electron or spin density
10. Show Electrostatic Potential: Open a dialog to control the visualization and calculation of molecular electrostatic potential (MEP)



**Figure 2.6.** Calculate menu.

The Calculate menu (Fig. 2.6) allow the user to change the GAMESS Input file options, submit a calculation to the PC GAMESS (if installed) and show/terminate any running GAMESS calculation.



**Figure 2.7.** Help menu.

The Help menu (Fig. 2.7) allows to run MaSK help and show the program information.

## 2.2 Toolbars

There is one status bar and 6 toolbars that can be shown or hidden through View menu (fig. 3) or by clicking with the right button of the mouse anywhere within the toolbar region. Some of the toolbars (all except Animation and Measuring) are the shortcuts to some of the menu options described previously in the Menu section. The following toolbars are available:

1. Standard
2. Animation
3. Formatting
4. Measuring
5. Editing
6. Results



**Figure 2.8.** Standard toolbar.

The Standard toolbar (Fig. 2.8) contains shortcuts to creating a new GAMESS Input file, opening existing file, saving opened GAMESS Input file and [converting](#) current file into new GAMESS Input file, printing image and Help.



**Figure 2.9.** Animation toolbar.

The Animation toolbar (Fig. 2.9) allows user to visualize all step of geometry optimization (if performed). The actions of each button are following:

1. Rewind to the initial geometry
2. Move to the previous geometry
3. Play all geometries in succession (turns into Stop button when activated)
4. Move to the next geometry
5. Fast forward to the last geometry



**Figure 2.10.** Formatting toolbar.

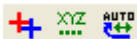
The Formatting bar (Fig. 2.10) allows user to zoom in or zoom out the molecule on the screen, as well as select the format of molecule presentation from Balls and Sticks, Spheres, Tubes, and Wireframe (see Molecule menu above). The last button allows to select/deselect the Hold & Pull Mouse option.



**Figure 2.11.** Measuring toolbar.

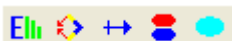
The Measuring toolbar (Fig. 2.11) allows the user to perform some measurements within a molecule. The actions of each button are following:

1. Clear all atom selections (e.g., from previous measurement).
2. Measure interatomic distance (need to select 2 atoms)
3. Measure angle (need to select 3 atoms)
4. Measure dihedral angle (need to select 4 atoms)
5. Measure interplanar angle (need to select 3+3 = 6 atoms where each triplet of points defines one plane).



**Figure 2.12.** Editing toolbar.

The Editing toolbar (Fig. 2.12) provides shortcuts to 3 options from the Edit menu (see above): Add Atoms/Groups, Modify Geometry, and Auto Resize/Recenter.



**Figure 2.13.** Results toolbar.

The Results toolbar (Fig. 2.13) provides shortcuts to 5 options from the Results menu (see above): Optimization Energy Graph, Calculated Vibrations, Show Dipole Direction, Show Molecular Orbitals, and Show Electron/Spin Density.





**Figure 2.14.** Status bar.

The Status bar at the bottom of the window (Fig. 2.14) provides information about which step optimization is currently visualized (if optimization has been performed) or reads Single-Point Calculation (if only one geometry was found in the file).

# 3. Molecule Visualization and Manipulation

## 3.1 Opening and Saving a File

In order to open an existing file, click on the  button on the Standard toolbar or select option Open from the File menu and then choose the file you want to open. If you want to save a file under a different name (available for GAMESS Input only), choose option Save As... from the File menu. To save a modified GAMESS Input file, press the  button.

When the molecule is initially opened, its size and position on the screen are automatically adjusted by the program to maximize the molecule's view on the screen: molecule's size is set to fill most of the screen and its orientation is such that most of the atoms are visible on the screen. The optimal initial orientation of the molecule on the screen is calculated only for molecules with 50 atoms or less.

## 3.2 Changing Molecule's Visualization Mode

If this is the first time you run MaSK, the molecule will be shown in its default *Balls and Sticks* visualization mode. Otherwise, the molecule will be shown in the mode that was selected in the last run of MaSK.

There are four molecule visualization modes available: Balls and Sticks, Spheres, Tubes and Wireframe. Each one can be selected through either a [Molecule menu](#) or by pressing a corresponding button on a [Formatting toolbar](#).



In *Balls and Sticks* mode, the atoms are presented as solid balls and bonds are presented as sticks. The radius of each ball depends on the atomic radius, which together with the radius of the bond (stick) can be modified in [Preferences](#). In the *Spheres* format, the atoms are presented as spheres whose radii depend on the Van der Waals radii that can be modified in [Preferences](#). When *Tubes* format is chosen, molecules are presented in the form of tubes whose ends and intersections represent atoms. The radii of the tubes for this format can also be modified in [Preferences](#). Finally, the *Wireframe* format is similar to the Tubes but lines are used instead of tubes.

## 3.3 Showing Additional Information

In addition to atoms and bonds visualized on the screen, user may choose to show/hide hydrogen bonds, atomic symbols and numbers. The coordinates axes may also be visualized. All these options are available from the [Molecule menu](#).





## 3.4 Zooming In/Out


The currently visualized molecule can be zoomed in (up to 200% view) or out (down to 25% view) using 3 methods:

1. Choose the zoom level directly from the Zoom drop down menu on the [Formatting toolbar](#).
2. Press  button to zoom in or  button to zoom out on the [Formatting toolbar](#).
3. Turn the mouse wheel (if present) towards you to zoom out or away to zoom in.

## 3.5 Measuring

There are four measuring tools available to user: distance between atoms, angle defined by 3 atoms, dihedral angle defined by 4 atoms, and interplanar angle defined by 6 (3+3) atoms. All these tools are available on the [Measuring toolbar](#).


1. Measuring distance. Press  button to measure the distance between two atoms (mouse cursor will turn into cross hair). Then, select two atoms in the molecules by clicking on the desired atoms. Selected atoms will be colored yellow.
2. Measuring angle. Press  button to measure the angle (mouse cursor will turn into cross hair) and then select 3 atoms. The selected atoms will be colored yellow.
3. Measuring dihedral (torsion) angle. Press  button (mouse cursor will turn into cross hair) and then select 4 atoms in a molecule. The selected atoms will be colored yellow.
4. Measuring interplanar angle. Press  button (mouse cursor will turn into cross hair) and select 3 atoms that define the first plane and then select 3 more atoms to define the second plane. All atoms must be unique. The selected atoms will be colored yellow.

After the required number of the atoms have been selected, the mouse cursor will return to the original state and the computed value will be displayed in the lower left corner of the window. To clear the selection, measured value or to cancel the measurement at any time, press the clear button () on the Measuring toolbar.

## 3.6 Molecule Manipulation

There are two ways to manipulate the molecule on the screen: using a mouse or keyboard.

There are 4 directional buttons on the keyboard that can be used to rotate the molecule up, down, left and right. The speed of rotation is slower than that for the mouse for a better precision.

There are two modes of using a mouse: regular and Hold & Pull. The modes can be switched by either pressing the  button on the [Formatting toolbar](#) or selecting Hold & Pull mouse from the [Molecule menu](#).






*Regular Mode.* With regular mode the screen is virtually divided into 9 equal squares (3 x 3). Pressing the left mouse button while keeping pointer in one of the squares (except the central one) rotates the molecule in that direction until the button is released. The central square is further divided into 4 triangles: top, bottom, left and right. Pressing the mouse button while keeping the mouse pointer in one of the triangles will rotate the molecule in the corresponding direction. The molecule can also be rotated clockwise on the screen if the right mouse button is pressed.

*Hold & Pull Mouse Mode.* In this mode, when the mouse is being moved while the left button pressed, the molecule is rotated in the direction of the mouse movement. In addition, pressing the right mouse button and moving mouse left or right allows to rotate the molecule counter- or clockwise, correspondingly.


## 4. Working with Output Files

### 4.1 Visualization of Optimization

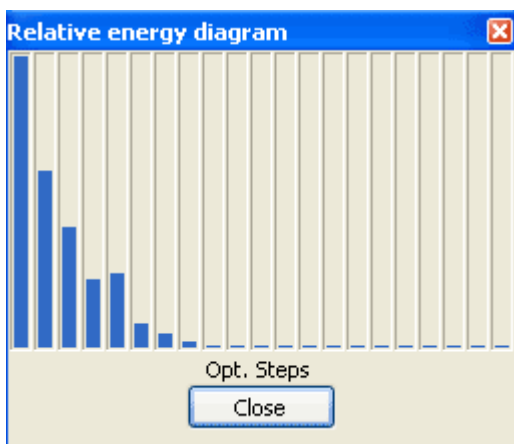
If the output file contains more than one geometry as in geometry optimization, saddle point localization or Intrinsic Reaction Coordinate (IRC) following, then all of the steps can be visualized as single steps or as an animation. When the output with multiple steps is first opened, either first (starting) or the last (optimized, if normally terminated) geometry is displayed depending on the user selection in [Preferences](#). The step number and the total number of geometries in the output file are displayed in the MaSK [status bar](#). The selection of the geometry to be visualized is done through the [Animation toolbar](#) or Optimization Energy Graph (see below).

There are five buttons available on the Animation toolbar: First () , Previous () , Animate () , Next () , and Last () . The First button causes the first geometry to be visualized (disabled if currently visualized geometry is the first one). The Last button causes the last geometry to be visualized (disabled if currently visualized geometry is the last one). The Previous and Next buttons go one step back or forward in the list of available geometries and are disabled if the first or last geometry are currently visualized, correspondingly. Finally, the Animate button causes to display all geometries (starting with the currently visualized) for a short duration until reaching the end. The duration of the display of each geometry can be customized in [Preferences](#).

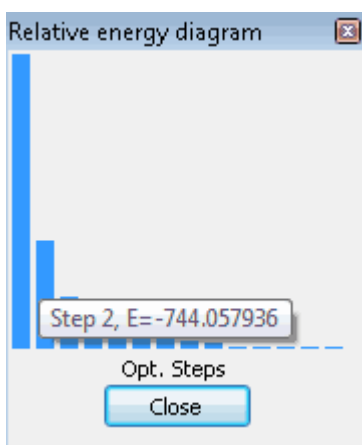
*Note:* for IRC calculations only optimized points on the reaction coordinate will be visualized for clarity.

The relative energies of each intermediate and final geometries can be compared by pressing the  button on the [Results toolbar](#) or selecting the optimization Energy Graph from the [Results menu](#) (Figure 4.1). Holding a mouse pointer over one of the columns representing the relative energies of each step will display the step number and the energy (in Hartree) for that step (Figure 4.2). In addition, left-click over any step in the graph will immediately visualize the selected step in main window. The full height of the diagram represents the difference between the largest and the smallest energy values among all steps.

*Note:* The visualized energies for Gaussian outputs are the SCF energies. If the calculations have been performed at the level other than Hartree-Fock or Density Functional Theory (DFT), consult the output file to locate the energies at the chosen level of theory.



**Figure 4.1.** Relative energy diagram (under Windows XP).



**Figure 4.2.** Relative energy diagram with mouse pointer (not shown) resting over second column (under Windows Vista).

## 4.2 Visualization of Molecular Properties


### 4.2.1 Dipole Moment

If the dipole moment has been correctly read from the output and the value is larger than 0, it can be visualized by pressing [+](#) button on the [Results toolbar](#) or selecting Show Dipole Direction from the [Results menu](#). Since the dipole shown is the one calculated for the last geometry (if more than one found), the last geometry will be visualized when this option is engaged.

### 4.2.2 Mulliken and Lowdin Charges

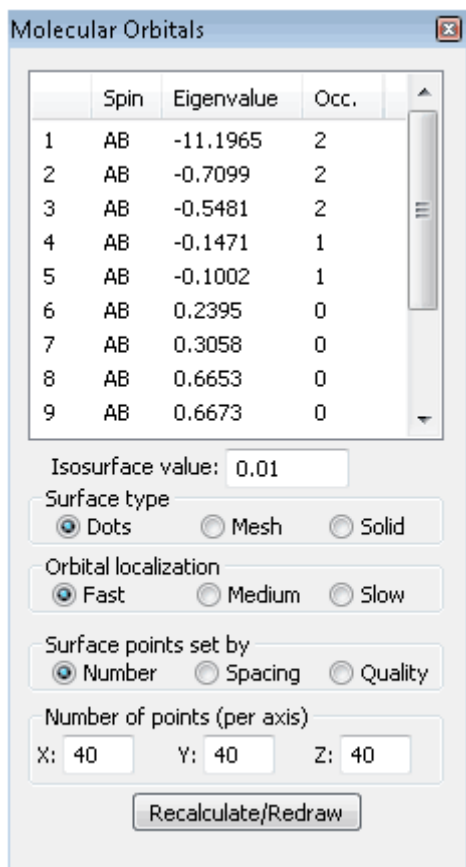
Calculated charges can be visualized by going to the [Results menu](#) and then Calculated Charges. Two options are available: Mulliken (Gaussian and GAMESS) and Lowdin (GAMESS only). These will show charges on each atom calculated according to Mulliken or Lowdin scheme, correspondingly. To hide charges, follow the same steps and deselect the currently displayed charges. *Note:* if the option is disabled, then the charges were either not calculated or not read correctly.

## 4.2.3 Molecular Orbitals

The molecular orbitals can be visualized by MaSK only if both atomic basis set and molecular orbital coefficients have been printed in the output file (see [Using MaSK with GAMESS](#) and [Using MaSK with Gaussian](#) for details). To open the Molecular Orbitals window, press the  button on the [Results toolbar](#) or select Show Molecular Orbitals from the [Results menu](#). Note: the option will be disabled if either atomic basis set or molecular orbital coefficients have not been found in the output file.

*Note:* When Orbitals window is open, the molecule format will be switched to Wireframe (can be changed after opening) for better visualization (especially for small orbitals, which can be hidden by the objects in other formats (i.e., balls, spheres, etc.)). If the output contains more than 1 geometry, then the last geometry will be visualized in the main window and Animation toolbar buttons will be disabled (so that the orbitals calculated for the last geometry would not be mapped on the wrong geometries).

Figure 4.3 below shows a sample Molecular Orbitals window.



**Figure 4.3.** Molecular Orbitals window.

There are several items and options shown in the Molecular Orbitals window: orbital list, isosurface value, surface type, orbital localization speed, surface points setting (and its suboption). Orbital list contains 4 columns: orbital number, spin, eigenvalue and occupancy. Spin values can be A (alpha), B (beta), and AB (combined alpha and beta) and indicate the spin of electron(s) on that orbital. Separate alpha and beta spins are available with unrestricted wavefunctions only. Occupancy show the number of electron occupying a particular orbital. The

list is sorted from lowest to highest eigenvalues. To visualize an orbital, simply click on a corresponding line in the list.

*Note:* To display the Highest Occupied Molecular Orbital (HOMO), select from the list the last orbital that has at least 1 electron on it (e.g., orbital #5 in Figure 4.3). To display the Lowest Unoccupied Molecular Orbital (LUMO), select from the list the first orbital without electrons (i.e., with 0 in the Occupancy column; e.g., orbital #6 in Figure 4.3).

*Iso*surface value allows to visualize the surface with a particular value of the wavefunction. The default isovalue is 0.01.

*Surface type* has three options: Dots (surface is represented as a series of points), Mesh (surface is represented as a series of lines connecting the points), and Solid (a solid surface is built). When Solid surface type is selected, an Opacity option will be shown at the bottom of the window that allows to change the opacity from completely transparent to completely opaque. *Note:* due to the nature of OpenGL transparency, some orbitals may not be visible through others and hidden sides of complex orbitals may be displayed incorrectly in a semitransparent mode.

*Orbital localization* allows to find the edges of the imaginary cube within which all orbital surface points are located. This, in turn, allows to not waste points for the space which is far from the actual orbital resulting in a smoother surface with smaller number of points. In order to localize the orbital, an initially large cube is chosen based on the coordinates of the atoms and then each side of it is moved inward step-by-step until the surface is intersected. With a *Fast* (default) or *Medium* options selected, MaSK first makes large steps, finds the edge of the orbital, steps back and then makes smaller steps to locate the orbital. With *Slow* option MaSK moves each side of the cube in small steps only. In addition, in *Slow* mode MaSK uses the same number of points per axis as in the final cube, while only half of the points is used in *Fast* and *Medium* modes.


*Note:* *Fast* option is appropriate for most orbitals. However, if after the calculation of the orbital is complete no orbital is displayed in the main window or the orbital has holes, then the orbital may be too small and was skipped due to very large steps or inadequate number of points selected. To correct this, either choose one of the better (albeit slower) *Orbital localization* options and/or increase the Number of points (see below).

*Surface points set by* allows to select the number of points that will be used for orbital visualization. More points (or less point spacing) increases the quality of the calculated orbital surface but significantly increases the time required for computations. The three options available are Number, Spacing, and Quality. If the points are set by *Number*, then the number of points per axis need to be selected. The default value is 40 points per axis. If the points are set by *Spacing*, then the spacing between points (in angstroms) needs to be selected. The default spacing is 0.10 angstrom. Finally, if the *Quality* option is selected, then the cube quality is defined by the number of points per angstrom. Options available for this type are Coarse, Medium, and Fine with 5, 10, and 20 points per angstrom, correspondingly.

Recalculate/Redraw button is needed only in the following two cases. 1. If the user changes some parameters described above and wants to redraw the currently visualized/selected orbital with new options. 2. If the orbital has been loaded from MaSK Cube File (for more on this, see Molecular Orbital Data in [Preferences](#)) and the user wants to recalculate it with new options.

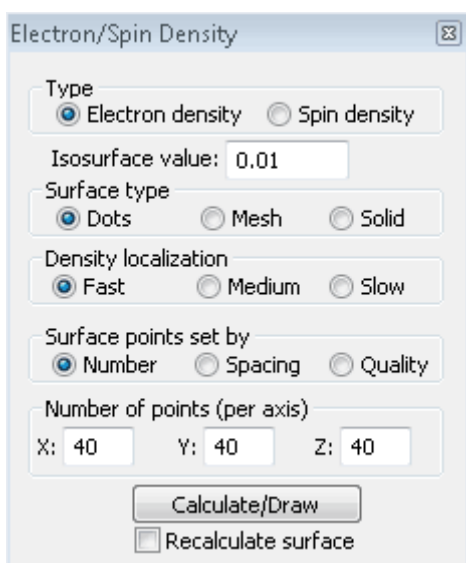
When new orbital is chosen for visualization or Recalculate/Redraw button is pressed, a progress bar will become visible below the Recalculate/Redraw button showing the progress of the orbital localization and calculation of the wavefunction values. The calculations may be cancelled at any time by pressing ESC button on the keyboard.

## 4.2.4 Electron and Spin Densities

The electron and spin densities can be visualized by MaSK only if both atomic basis set and molecular orbital coefficients have been printed in the output file (see [Using MaSK with GAMESS](#) and [Using MaSK with Gaussian](#) for details). To open the Electron and Spin Density window, press the  button on the [Results toolbar](#) or select Show Electron/Spin Density from the [Results menu](#). Note: the option will be disabled if either atomic basis set or molecular orbital coefficients have not been found in the output file.

*Note:* When Electron/Spin Density window is open, the molecule format will be switched to Wireframe (can be changed after opening) for better visualization. If the output contains more than 1 geometry, then the last geometry will be visualized in the main window and Animation toolbar buttons will be disabled (so that the density calculated for the last geometry would not be mapped on the wrong geometries).

Figure 4.4 below shows a sample Electron/Spin Density window.



**Figure 4.4.** Electron/Spin Density window.

The options available in the Electron/Spin Density are mostly the same as in the Molecular Orbitals window (see above). Select Electron density or Spin density radio button in the Type group to build electron or spin density, correspondingly. See the description of the other options available (Isosurface value, Surface type, etc.) in the [Molecular Orbitals](#) section.

After all options have been set, press the Calculate/Draw button to calculate and draw the selected density. The progress bar will show the current progress in localizing density, calculating density values and drawing surface (press ESC at any time to cancel the operation).

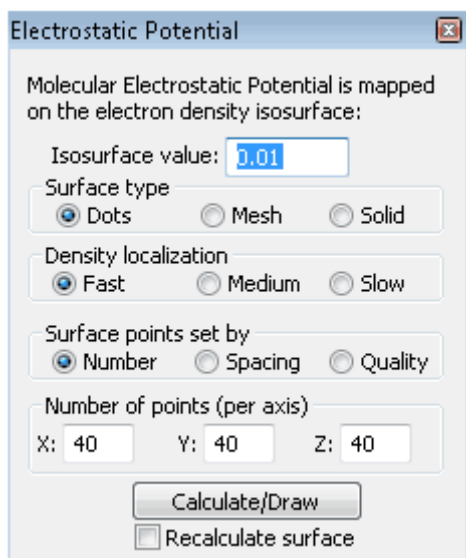
If the electron or spin density has been previously saved to the MaSK Cube File and current user setting is to Save Calculated Cube Data to File (for more on this, see Molecular Orbital Data in [Preferences](#)), the data will not be calculated and will be loaded from the file. If you want to force the new calculation, check the *Recalculate surface* option below the Calculate/Draw button and press the latter.

## 4.2.5 Molecular Electrostatic Potential

The Molecular Electrostatic Potential (MEP) can be mapped onto electron density and visualized by MaSK only if all three of the following data is printed in the output file: 1) atomic basis set, 2) molecular orbital coefficients, and 3) Mulliken atomic charges (see [Using MaSK with GAMESS](#) and [Using MaSK with Gaussian](#) for details). To open the Molecular Electrostatic Potential window, select Show Electrostatic Potential from the [Results menu](#). Note: the option will be disabled if any of the aforementioned data have not been found in the output file.

*Note:* When Electrostatic Potential window is open, the molecule format will be switched to Wireframe (can be changed after opening) for better visualization. If the output contains more than 1 geometry, then the last geometry will be visualized in the main window and Animation toolbar buttons will be disabled (so that the density calculated for the last geometry would not be mapped on the wrong geometries).

Figure 4.5 below shows a sample Electrostatic Potential window.




**Figure 4.5.** Electrostatic Potential window.


Since the electrostatic potential is mapped on the electron density surface, you must select the isovalue for that surface. For the description of available options see [Electron and Spin Densities](#) and [Molecular Orbitals](#) sections.

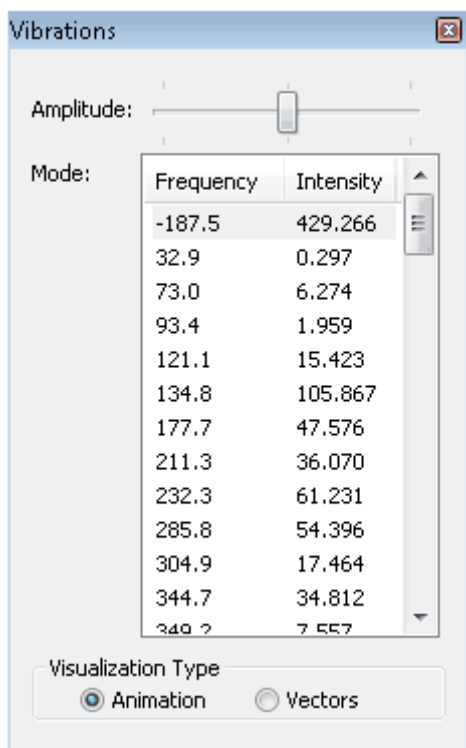
After the MEP is displayed, the color scale with the smallest, medium and largest values of the potential (in  $\text{electron}^2/\text{Bohr}$ ) is displayed in the lower-left corner of the main window.

If the electron density with the same isosurface value as currently selected has been previously saved to the MaSK Cube File and current user setting is to Save Calculated Cube Data to File (for more on this, see Molecular Orbital Data in [Preferences](#)), the electron density will not be calculated and will be loaded from the file. If you want to force the new calculation of the density, check the *Recalculate surface* option below the Calculate/Draw button and press the latter.

## 4.3 Visualization of Molecular Vibrations

If the calculations of the vibrational frequencies have been performed and the results have been printed in the output file, they can be visualized in MaSK by either pressing  button on the [Results toolbar](#) or selecting *Calculated Vibrations* from the [Results menu](#). Both the button and the menu option will be disabled if the vibrational frequencies have not been found in the output file.

After the  is pressed or *Calculated Vibrations* menu option is selected, a Vibrations window (see Figure 4.6) will be open.



**Figure 4.6.** Sample Vibrations window.

The Mode window contains all calculated harmonic vibrational frequencies (in  $\text{cm}^{-1}$ ) and corresponding IR intensities (KM/Mole, Gaussian;  $\text{Debye}^2/\text{amu}\cdot\text{Angstrom}^2$ , GAMESS). The list is sorted by increasing frequency value. Selecting any mode in the list will display the corresponding vibrational mode in the main window with either animation (if Visualization Type is set to Animation) or vectors (if Visualization Type is set to Vectors).

*Note:* It is recommended to switch to Wireframe molecular format when visualizing vibrations in the form of vectors as some vectors may be hidden by balls/spheres representing atoms and/or cylinders representing bonds.

The amplitude of the animated vibration or the size of the vector can be increased or decreased by sliding the *Amplitude* control to the right or to the left of the center. The rate of the animated vibration can be regulated through the *Rate of Vibration* in [Preferences](#).

## 4.4 Viewing Result Summaries

Instead of searching for basic information through the output file, Result Summaries (brief and extended) can provide most of the required data in a concise form. To view the summary, select Brief Summary (or Extended Summary) from the [Results menu](#).

Brief summary provides the following information: type of calculations, method, basis set, stoichiometric formula, number of atoms in the molecule, multiplicity, charge, dipole moment, final energy (except for IRC calculations). In addition, for geometry optimization and saddle point (transition state) localization calculations, the number of steps will be printed with the information whether the optimization/localization was completed.



Extended summary adds the following information to the brief summary where calculated: thermochemical data (temperature, zero-point energy (ZPE), entropy, total electronic and thermal energy, enthalpy and Gibbs free energy, etc.), energy for each step of optimization/saddle point localization/IRC following, calculated Mulliken (GAMESS and Gaussian) and Lowdin (GAMESS) charges for all atoms, potential energy surface scan results (GAMESS only).

## 4.5 Exporting PES Scan Result (GAMESS)

Results of the Potential Energy Surface (PES) scan performed by GAMESS can be exported to the Comma-Separated Values (CSV) file for further use in the graph-building capable software (e.g., Microsoft Excel). When PES scan results are detected in GAMESS output, an extra option Export PES Results... will be added at the bottom of the [Results menu](#). Selecting this option will bring up a dialog to select a file name and location for the CSV file. *Note:* only completed PES scan results can be exported.

# 5. Converting Output to Input

Unless the file opened is GAMESS input, the geometry cannot be modified and saved (Gaussian input can be modified but cannot be saved). Converting the file into GAMESS input allows user to modify geometry and save it. Gaussian input, Gaussian output and GAMESS output files can be easily converted to GAMESS input in several ways:

1. If working with Gaussian input or single-point GAMESS/Gaussian output calculations, user can convert it to GAMESS Input by pressing  button or save a file as GAMESS Input by choosing Save As... from File menu.
2. If working with GAMESS or Gaussian output files containing several geometries (e.g., geometry optimizations), then select the geometry that you want to modify (e.g., by visualizing the desired optimization step) and after that convert it to GAMESS Input by pressing  button or save that geometry as GAMESS Input by choosing Save As... from File menu.




In both cases the default GAMESS input option will be given to the newly created input files.

## 6. Working with Input Files

Only GAMESS Input files can be modified. See [Converting Output to Input](#) section on instructions about converting other formats into GAMESS Input.

Note: when no file is open or New button is pressed on the [Standard Toolbar](#), the file format is automatically set to GAMESS Input.

All geometry modification options are accessed through three buttons on the [Editing Toolbar](#).

The functions of these buttons are Add atoms () , Modify geometry () , and Reset molecule's size/position () . The latter simply resizes and repositions the molecule such that its center coincides with the center of the window and all atoms fit in the MaSK window and is useful when building a new molecule or adding atoms or groups to existing one.


In addition to adding atoms or modifying geometry, user can also set/change GAMESS input options and run GAMESS calculations without leaving MaSK.

You may

1. [Modify geometry](#)
2. [Add atoms](#)
3. [Add groups of atoms](#)
4. [Set GAMESS input options](#)
5. [Run GAMESS calculations](#)

### 6.1 Modifying Geometry

The geometry of any molecule can be given by different means of which most common are Z-Matrix and Cartesian coordinates. Z-Matrix defines a molecule through an atomic connectivity or simply their positions relative to other atoms. For example, every atom (except the first one) has another atom to which it is bonded (or simply defined through) and the distance to that atom. The same way the angle and the dihedral angle are given. Cartesian coordinate method, on the other hand, does not use atomic connectivity. It simply defines the position of each atom in space by giving the values of x, y, and z coordinates.

The geometry of an existing molecule can be modified in MaSK through either Z-Matrix (Fig. 6.1) or Cartesian coordinates of atoms (Fig. 6.2). Press  button to bring up a *Modify geometry* dialog. To switch between Z-Matrix and Cartesian, press the corresponding tab in the dialog.

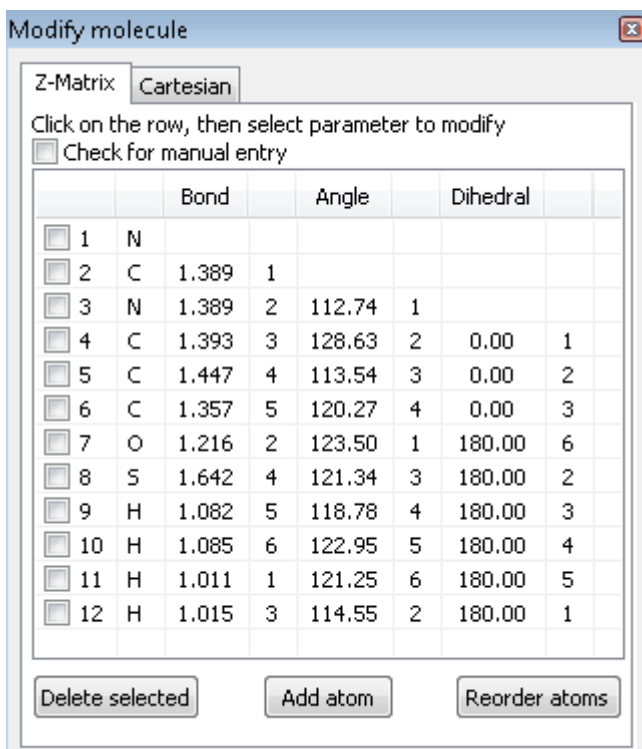


Figure 6.1. Z-Matrix page of the Modify molecule dialog.

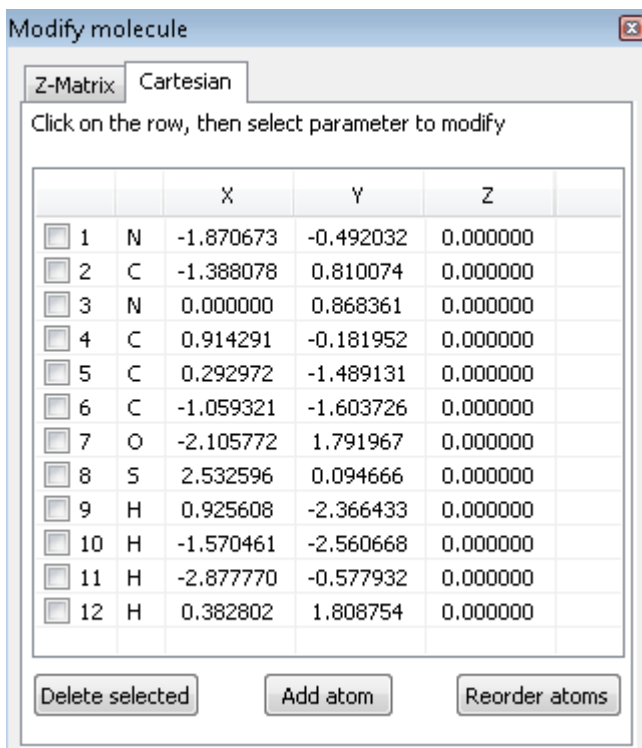


Figure 6.2. Cartesian page of the Modify molecule dialog.

The Z-Matrix of the molecule is represented using 8 columns: 1) ordinal number of the atom in a molecule, 2) atomic symbol, 3) bond length (in Å), 4) bond connectivity atom number, 5) angle (in degrees), 6) angle connectivity atom, 7) dihedral angle (in degrees), 8) dihedral angle

connectivity atom. The first three atoms in each molecule do not have all 8 parameters. The first atom in the Z-Matrix has only first two, the second one has four, and the third one has six columns filled.

The Cartesian coordinates are displayed using 5 columns: 1) ordinal number of the atom in a molecule, 2) atomic symbol, 3) X-coordinate, 4) Y-coordinate, and 5) Z-coordinate.

To modify any value in Z-Matrix (columns 2 through 8) or Cartesian coordinates (columns 2 through 5), first click on the row for the atom which value you want to modify (the selected atom will change color to yellow in the main window) and then click on the value you want to modify. The field will then change to editable text box. After new value is entered, press ENTER or simply leave the field by clicking outside the value area to apply the change or press ESC to cancel the change.


GAMESS allows to freeze some bonds/distances to perform a restricted optimization. If such optimization is desired, right-click the bond(s) you want to freeze and select Freeze from the pop-up menu. The frozen distance will be colored in red. To unfreeze, right-click the value and select Unfreeze from the pop-up menu.

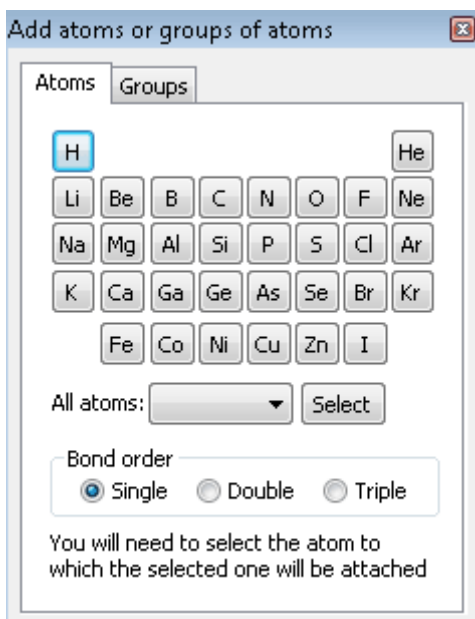
To delete atoms, select all atoms you wish to delete by checking the boxes for those atoms and press the *Delete selected* button. If some of the deleted atoms were used as connectivity for other atoms, then new connectivity atoms and values will be selected automatically and the positions of the remaining atoms will be preserved.

To change the order of the atoms in the molecule, press the *Reorder atoms* button. When the latter is pressed, the dialog will disappear and mouse pointer will change to cross-hair. You now have to click on every atom in the molecule to select them in the order you want the atoms to be ordered in a molecule. All selected atoms will be colored in yellow until the last atom is selected or reordering cancelled. After the last atom is selected or reordering is cancelled the *Modify geometry* dialog window will show up automatically and the mouse pointer will change back to normal.

To add atoms or groups of atoms to the molecule, press the *Add atom* button (for more information, read the following sections [Adding Atoms](#) and [Adding Groups of Atoms](#)).

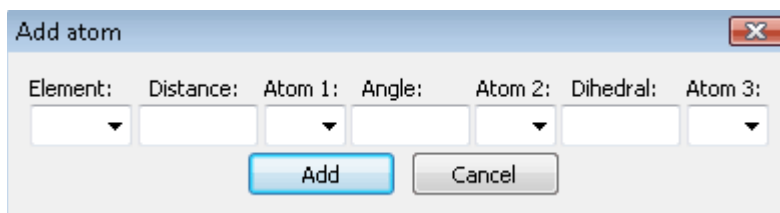
## 6.2 Adding Atoms

There are two ways to add atoms, automatic and manual. To add atoms automatically, press  on the Editing toolbar or press *Add atom* button in the *Modify molecule* dialog (make sure the checkbox for manual entry at the top of the Z-Matrix is unchecked). The *Add atoms or groups of atoms* dialog will appear (Fig. 6.3). To add atom to the molecule, press the corresponding button on a brief version of the periodic table or select an atom from a drop-down list and press the *Select* button next to it. After that the dialog will disappear and you will need to select an atom to which the selected atom will be attached (except for the first atom in the molecule, which will be added right away). When the atom is clicked, the new atom will be attached to it with a distance that depends on the *Bond order* selected in the dialog. The angle and dihedral angle values as well as the connectivity atoms will be chosen automatically and can be later modified through a *Modify geometry* dialog (see above).



**Figure 6.3.** The Atoms page of the Add atoms or groups of atoms dialog.


Manual addition of atoms allows you to set all connectivity atoms and the values of distance, angle and dihedral angle manually. To add atoms manually, press *Add atom* button in the *Modify molecule* dialog with a checkbox for manual entry at the top of the Z-Matrix checked. The *Add atom* (Fig. 6.4) dialog will appear.

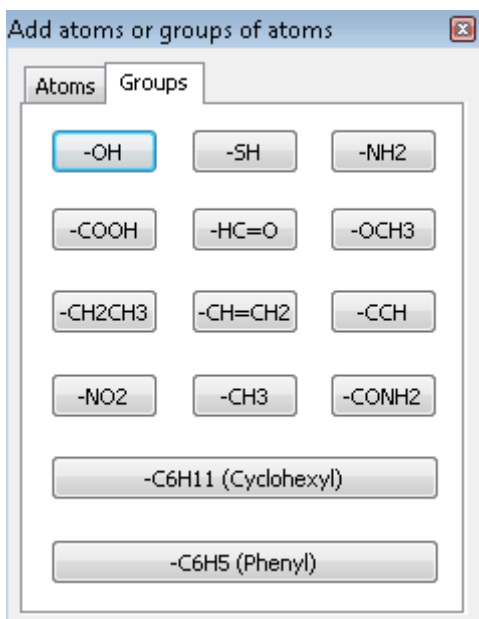


**Figure 6.4.** The Add atoms dialog for manual atom entry.

Depending on the current number of atoms in a molecule, some of the fields may be disabled. If adding the first atom in the molecule, then only the Element drop-down list will be available. If adding the second atom, then enter the distance in the Distance textbox and select the Atom 1 from the drop-down list of all atoms in the molecule in addition to selecting the element being added. For third atom one needs to also enter the angle value and select the second atom from the list of all atoms in a molecule. The fourth and further atoms require all fields to be filled. *Note:* all connectivity atoms must be unique; when choosing connectivity atoms you cannot select the same atom more than once (you will get an error message if you do).

## 6.3 Adding Groups of Atoms

To add groups of atoms, press  on the Editing toolbar or press *Add atom* button in the *Modify molecule* dialog (make sure the checkbox for manual entry at the top of the Z-Matrix is unchecked). When the *Add atoms or groups of atoms* dialog appears (Fig. 3), press the Groups tab at the top of the dialog. There are 14 pre-built functional groups available for automatic addition to the molecule (Fig. 6.5).

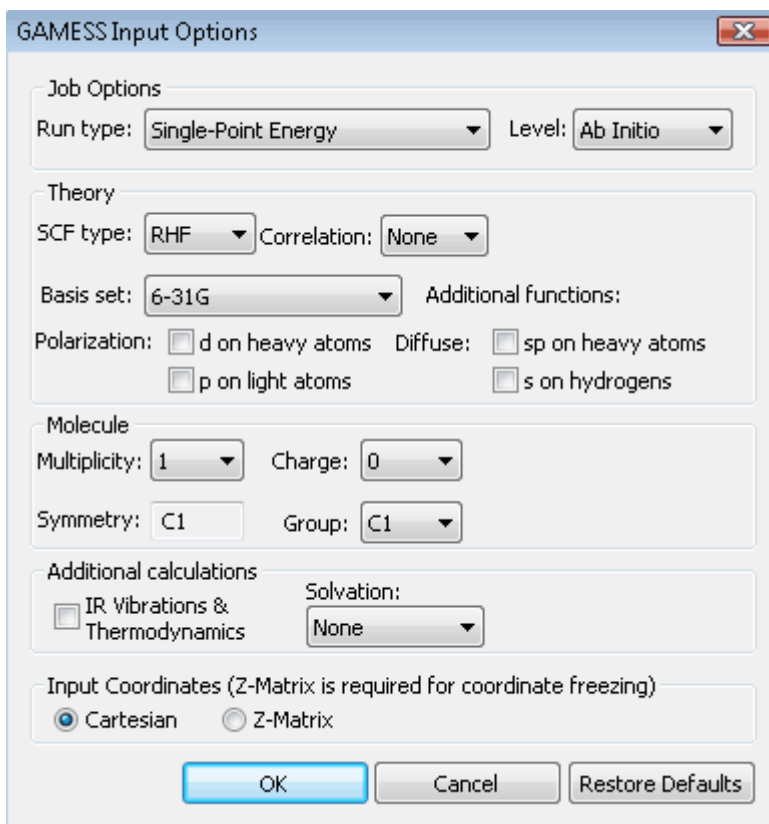


**Figure 6.5.** Add Groups page of the *Add atoms or groups of atoms* dialog.

To add a group, press the corresponding button on the page. After the group is selected, the dialog will disappear and an atom in the molecule to which the new group will be attached should be selected.

## 6.4 Setting GAMESS Input Options

When GAMESS input file is initially created, it is automatically assigned default input options (see Fig. 6.6). To change the options, select Input Options from the Calculate menu.



**Figure 6.6.** GAMESS Input Options dialog with default options.

The dialog contains some most frequently used options. Following are the list of available options for each property.

**Run type:** Single-Point Energy, Geometry Optimization, Transition State, Potential Energy Surface. This sets the type of calculation to be performed. Geometry optimization and Transition State are the localizations of local minimum and saddle point (transition state), correspondingly.

**Level:** Ab Initio, MNDO, AM1, PM3. The last three options are semiempirical methods.

**SCF Type:** RHF, UHF, ROHF. Sets a type of self-consistent field (SCF) to Restricted Hartree-Fock (RHF), Unrestricted Hartree-Fock (UHF), or Restricted Open-Shell Hartree-Fock (ROHF).

**Correlation:** None, MP2, DFT. Sets the correlation level to none, Moller-Plesset Second Order Perturbation (MP2) or Density Functional Theory (DFT) level.

**DFT Type:** B3LYP1, B3LYP5, BHHLYP, BLYP, LYP, BVWN5. Selects the functional for DFT calculations (available when DFT correlation is chosen).

**Basis set:** STO-3G, 3-21G, 6-31G, 6-311G, Double-zeta valence, Triple-zeta valence. The first basis set is the Pople's minimal basis set. Basis sets 2-4 are the standard split-valence Pople's basis sets. The last two are Dunning's correlation consistent double-zeta and triple-zeta basis sets. Some basis sets allow to add polarization functions (on heavy and/or light atoms) and diffuse functions (on heavy and/or hydrogen atoms). Consult GAMESS manual to find which basis sets allow polarization and/or diffuse functions added to them.

Molecule's specifications include Multiplicity (1-5), Charge (-3...0...+3), and Symmetry Group.

Additional calculation options include IR Vibrations and Thermodynamics (to calculate vibrational frequencies and various thermodynamic data) and Solvation. If solvation is chosen, then the solvent must also be selected.

Finally, the input coordinates may be saved as either Cartesian coordinates or Z-Matrix.

If the run type is set to Potential Energy Surface (PES), then additional options will be available in the dialog (see Fig. 6.7). In GAMESS you may build a one-dimensional PES by varying a single distance or two-dimensional PES by varying two distances. In the Distance #1 area select atoms 1 and 2, between which the distance will be varied. The original distance and the final distance values will be automatically filled with current distance values in the molecule. Modify original or final distance (or both) and select the number of steps you want to be calculated on the PES. The step size will be automatically calculated based on your values. Repeat procedure for the Distance #2 if two-dimensional PES is desired (leave Distance #2 values at their defaults settings if only a single-dimensional PES is desired).

The screenshot shows the 'GAMESS Input Options' dialog box. The 'PES Options' section is active, showing two distance settings. Distance #1 is configured for atoms O1 and H2, with an original distance of 1.0100 Å and a final distance of 1.4100 Å, over 4 steps with a step size of 0.1000 Å. Distance #2 is configured for atoms O4 and H5, with an original distance of 1.0100 Å and a final distance of 1.6100 Å, over 6 steps with a step size of 0.1000 Å. The dialog also includes sections for Job Options (Run type: Potential Energy Surface, Level: Ab Initio), Theory (SCF type: RHF, Correlation: None, Basis set: 6-31G), Molecule (Multiplicity: 1, Charge: 0, Symmetry: C1, Group: C1), Additional calculations (Solvation: None), and Input Coordinates (Cartesian selected).

Figure 6.7. PES options on the GAMESS Input Options dialog.

Options presented in this dialog are only a very small subset of all options available in the PC GAMESS. If the option you would like to set is not available through this dialog, then you need to modify the input file manually (consult PC GAMESS manual for details).

## 6.5 Running GAMESS Calculations

To run GAMESS calculation from within MaSK, do the following:

1. Open GAMESS Input file (or convert other format into GAMESS Input).
2. Modify GAMESS input options as described in previous section (only if needed).
3. Select *Run Calculations* from the Calculate menu.

You will then be prompted for the name of the file to which the GAMESS output will be saved.

*Note:* If this is the first time you are trying to run PC GAMESS from MaSK, you will be asked to choose the location of the GAMESS.EXE file on your computer.


To see if the GAMESS calculation is running, choose *Show Running Calculations* from the Calculate menu. If the calculation is running, the window will show the names of the input and output files. Click on *Terminate* button if you want to terminate the calculation. *Note:* the status is updated only when the window is first open; to update the status press the *Refresh* button.

## 7. Saving, Printing and Copying Images

### Saving Images

All images generated by MaSK can be saved in one of the four formats: JPEG, GIF, BMP and PNG. The size of the resulting graphics file can be changed in [Preferences](#). In order to save the image that is currently in the main window, select option *Save Image As...* from the File menu. You will then be asked to select a name (the default name is that of the currently open file), location and the format for the saved graphics file.

### Printing and Copying to Clipboard

In addition to saving the image, it can also be printed (if at least one printer is available) or copied to clipboard. *Note:* no matter what color background is currently chosen, the image will be printed without background (equivalent to white background if printed on white paper). In order to print, press the  button on the [Standard toolbar](#), select *Print* from the File menu or press Ctrl-P.

To copy the image to clipboard, either press Ctrl-C or select *Copy to Clipboard* from the Edit menu. The size of the copied image and its resolution depend on the resolution of the monitor. If higher size/resolution is desired, then saving the image into file is recommended (see above).

## 8. Exporting Cartesian Coordinates

Cartesian coordinates of the visualized molecule can be exported into a text file for use in an application other than GAMESS. In order to do that, visualize the geometry you want to export (e.g., visualize a desired step of optimization) and then choose option *Export Cartesians...* from the File menu. You will then be able to choose the name and location of the file containing Cartesian coordinates.

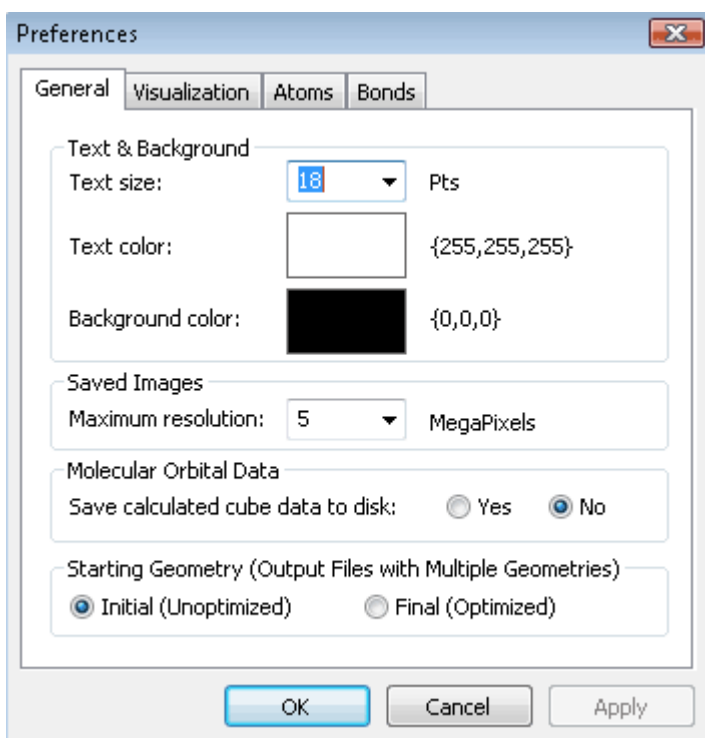
# 9. Customizing MaSK

There are several parameters that a user can customize in MaSK. All customizable parameters can be accessed by selecting a Preferences option in the Edit menu. *Note:* all customizations are user-specific, which means that every user account on the same computer will have its own customized options.

The Preferences dialog has four tabs: General, Visualization, Atoms, and Bonds. Following sections contain the description of the options available on each page in the Preferences dialog.

## 9.1 General

Use this page (Fig. 9.1) to change the size of the on-screen text, color of the text and background, maximum resolution of the saved images, and options to save calculated molecular orbital data (cube) to disk and whether to start from the initial or final geometry when opening an output with multiple geometries.



**Figure 9.1.** General page of the Preferences dialog.

The Text size option controls the size of the on-screen text used for displaying atomic labels, charges, as well as measured parameters such as distance, angle, etc. The size range is from 9 to 36 pts.

The color boxes for the text color and background color display the currently selected colors and the corresponding RGB values are displayed in the curled brackets. Text color and background color can be changed by clicking on the corresponding color box, which will bring up a color dialog.

The maximum size/resolution of the saved image (in MegaPixels, or MP) can be set by choosing a size from a *Maximum resolution* drop-down menu. Available options include 1, 2.5, 5, 10, and 20 MP. The size is defined as the product of picture's height and width in pixels. Note: this setting sets the approximate size of the picture; the actual size of the picture will vary depending on the proportions of the program window.

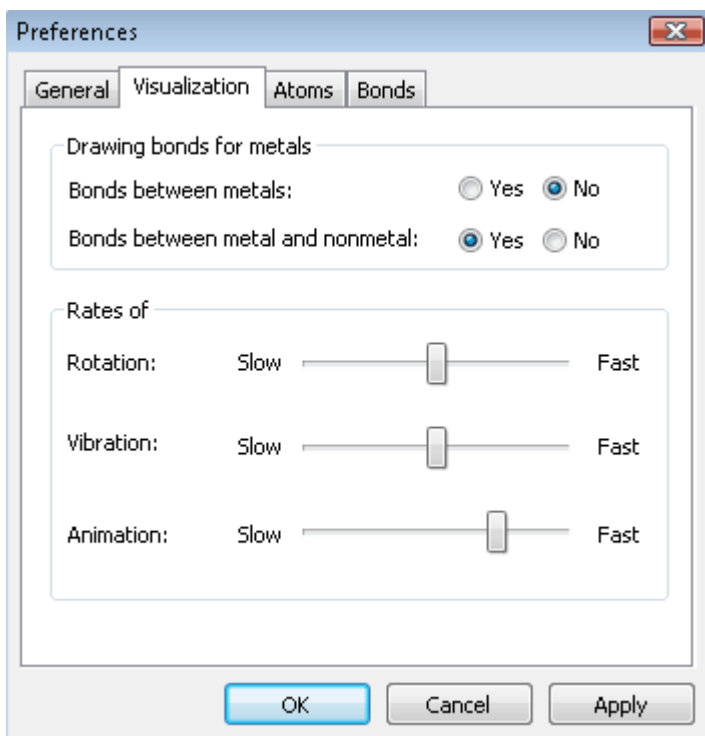
When building surfaces such as [molecular orbitals](#) and [electron density](#), a large amount of data is being calculated. In order for the MaSK to not recompute those values each time the desired surface is visualized, the calculated data (cube data) can be saved to file. If this option is selected, each time a surface is calculated the values will be saved to a MaSK Cube file, which will have the same name as the currently open output file with an .mcu file extension. In addition, when this option is selected, each time a surface is being built the MaSK will check if this surface has been previously calculated and save into MaSK Cube file. If found, the data will be loaded from file and no additional calculations will be performed.

*Note:* the more surfaces are saved into a MaSK Cube file, the more time it takes to search for a particular cube data in this file. Therefore, it is recommended to turn this option off when visualizing a large number of surfaces for the same molecule, especially if the molecule and/or the basis set are small (in other words, when calculations are faster than file reading).

When MaSK opens an output file with multiple geometries (i.e., geometry optimization, saddle point localization, IRC, etc.), either first or last geometry will be displayed depending on the option chosen by the user. The default setting is to display the initial geometry. To change the starting geometry to final, choose the Final (Optimized) option for the Starting Geometry setting.


## 9.2 Visualization

The Visualization page (Fig. 9.2) allows to set options for drawing bonds between two metals and between metals and nonmetals, as well as change the rates of rotation, vibration, and animation.



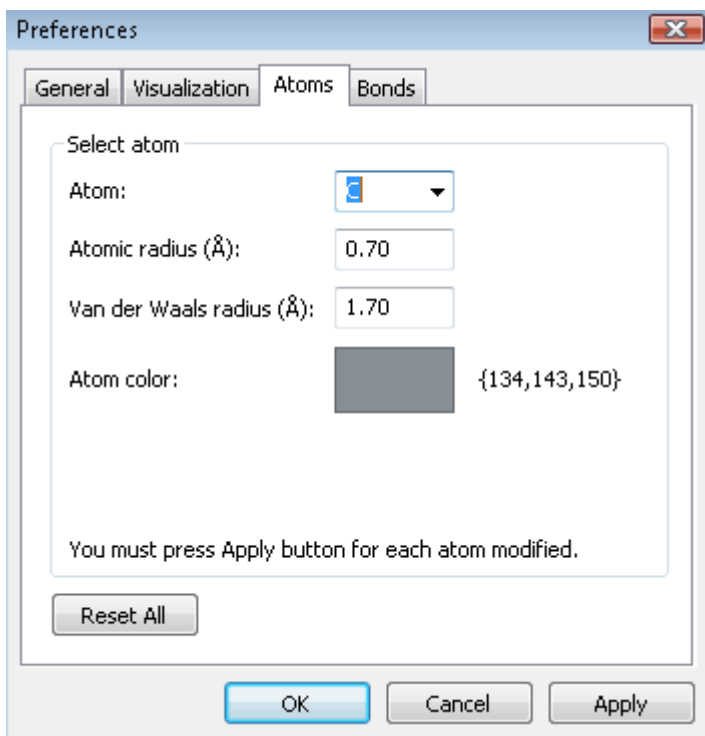
**Figure 9.2.** Visualization page of the Preferences dialog.

To change any of the three rates, move the slider towards Slow (for slower rate) or towards Fast (for faster rate).

The rate of Rotation controls how fast the molecule will be rotated when left button of a mouse is pressed while in [regular mouse](#) mode (not Hold & Pull mouse). The rate of Vibration controls how fast the atoms will be shifted while the molecular vibrational modes are displayed. Finally, the rate of Animation determines how long each step will be displayed in multiple-geometry outputs when the [Animate button](#)  is pressed. *Faster* setting means shorter duration for each step.

## 9.3 Atoms

The Atoms page (Fig. 9.3) allows to change some atomic parameters such as atomic radius, Van der Waals radius and color.



**Figure 9.3.** Atoms page of the Preferences dialog.

Atomic radius determines the radius of the balls in the [Balls and Sticks](#) visualization mode. The radii of the balls for all atoms except hydrogen in this mode scaled to 60% of the atomic radii. The radius of the hydrogen atom is set to 72% of the hydrogen's atomic radius.

Van der Waals radius determines the radius of the sphere representing atom in the [Spheres](#) visualization mode. Van der Waals radii are not scaled.

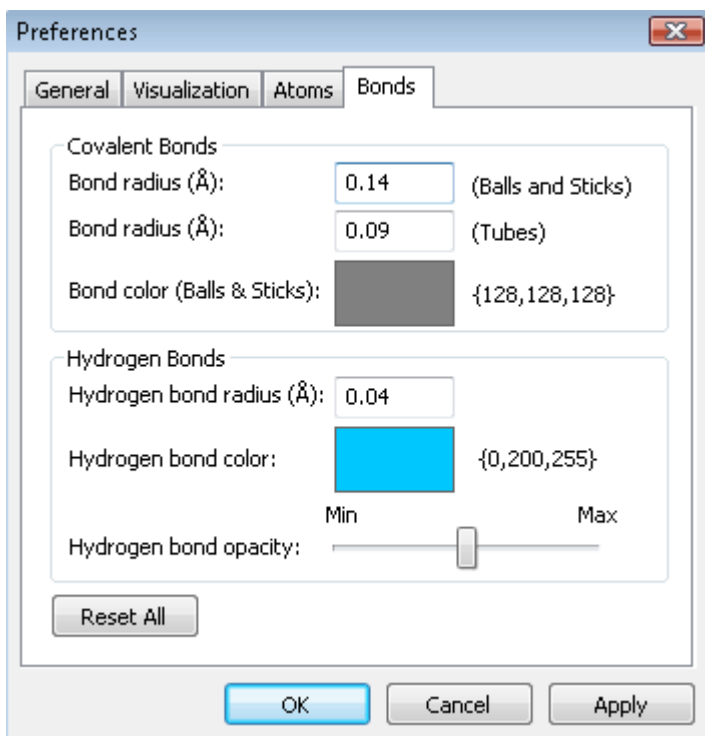
*Note:* In addition to determining the radii of the balls on the screen, the atomic radius is also used in determining whether a bond exists between two atoms. The bond is drawn if the distance between atoms is less than 125% of the sum of their atomic radii.

Each atom's color can be changed by left-clicking on the color box and selecting a new color. The color shown in the color box represents the currently set color for a selected atom.

To change any values for a particular atom, first select a desired atom from a drop-down list, change the values of radii and/or color and then press Apply (or OK) button. To reset all customized values for all atoms to their default values, press Reset All button.

## 9.4 Bonds

The Bonds page (Fig. 9.4) allows to change the values of the covalent and hydrogen bond radii as well as their color and opacity (for hydrogen bonds only).



**Figure 9.4.** Bonds page of the Preferences dialog.

There are two covalent bond radii present on this page. The first one determines the radius of the bond in the [Balls and Sticks](#) visualization mode, while the second one is for the [Tubes](#) mode. The default value of the bond radius in Balls and Sticks model is 0.14Å, which is approximately 80% of the default radius of the ball representing hydrogen atom. The default value of the bond radius in Tubes model is 0.9Å, which is approximately 50% of the default radius of the ball representing hydrogen atom.

The hydrogen bond radius is set by default to 0.04Å, which is approximately 20% of the default radius of the ball representing hydrogen atom.

The hydrogen bond opacity determines how opaque the hydrogen bond will look on the screen. The values range from Min (completely transparent) to Max (completely opaque).

The colors of covalent bonds currently selected are displayed in the corresponding color boxes. To change the color, click on the box and select a new color.