Gabedit

Version 2.1.0

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http://gabedit.sourceforge.net

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1) What is Gabedit ?

Gabedit is a graphical user interface to computational chemistry packages like Gamess-US, Gaussian, Molcas, Molpro, MPQC PCGamess and Q-Chem

It can display a variety of calculation results including support for most major molecular file formats. The advanced "Molecule Builder" allows to rapidly sketch in molecules and examine them in 3D. Graphics can be exported to various formats, including animations.

Major features

- Gabedit can creates input file for GAMESS(US), GAUSSIAN, MOLCAS, MOLPRO , MPQC PCGamess and Q-Chem.
- Gabedit can graphically display a variety of Gamess-US, Gaussian, Molcas, Molpro, MPQC, PCGamess, Q-Chem and (partially) ADF calculation results, including the following
    - Molecular orbitals.
    - Surfaces from the electron density, electrostatic potential, NMR shielding density, and other properties.
    - Surfaces may be displayed in solid, translucent and wire mesh modes. they are can be colorcoded by a separate property.
    - Contours (colorcoded), Planes colorcoded, Dipole. XYZ axes and the principal axes of the molecule.
    - Animation of the normal modes corresponding to vibrational frequencies.
    - Animation of the rotation of geometry, surfaces, contours, planes colorcoded, xyz and the principal axes of the molecule.
    - Animation of contours, Animation of planes colorcoded.
- Gabedit can display UV-Vis, IR and Raman computed spectra.
- Gabedit can generate a povray file for geometry (including hydrogen's bond),surfaces (including colorcoded surfaces), contours, planes colorcoded.
- Gabedit can save picture in BMP, JPEG, PNG, PPM and PS format.
- Gabedit can generate automatically a series of pictures for animation (vibration, geometry convergence, rotation, contours, planes colorcoded).

2) Platforms

Gabedit is pretty much platform independent. Up to now It has tested on Windows(XP, 2000, Vista), Linux (RedHat, Mandrake, Debian), MacOSX and UNIX (Digital TRU64, **Sun** Ultra, IBM AIX....)

Gabedit is written in C and uses the gtk+ and OpenGL (or Mesa3D) libraries.
Please note : the 2.4.x (or higher) version of Gtk+ is required for this version of Gabedit.
The gtk+ and OpenGL(or Mesa3D) graphics libraries are available on many UNIX systems, LINUX and also on WINDOWS.

3) Availability

Gabedit is free. The source files are available. Precompiled executable files are available for Linux, Mac OS X11 and Windows systems.

4) Citation

Please use the following citations in any report or publication :

A.R. ALLOUCHE, Gabedit is a free Graphical User Interface for computational chemistry packages. It is available from http://gabedit.sourceforge.net/

5) License

6) Installation

6-1 Requirements

OpenGL (or Mesa3D) and gtk+.2.4.x (or higher) libraries for UNIX.
Nothing for Linux, MacOSX11 and Windows system.

6-2 Unpack and install under Linux (and UNIX) system using the source files

download Gabedit210Src.tar.gz file from http://gabedit.sourceforge.net/
Execute the following commands:

```
gunzip    Gabedit210Src.tar.gz
tar  -xvf    Gabedit210Src.tar
cd   Gabedit210Src
make
/gabedit
```

6-3 Unpack and install under Linux system using the binary files

6-3-1 Gtk2+ is installed in your system

download Gabedit207LinuxI386Glibc23.gz from http://gabedit.sourceforge.net/
Execute the following commands:

```
gunzip   Gabedit210LinuxI386Glibc23.gz
cp  Gabedit210LinuxI386Glibc23 gabedit
chmod u+x gabedit
./gabedit
```

6-3-2 Gtk2+ is not installed in your system

download Gabedit210LinuxI386Glibc23IncludingGTKLib.tar.gz

Execute the following commands:

```
gunzip   Gabedit210LinuxI386Glibc23IncludingGTKLib.tar.gz
tar -xvf Gabedit210LinuxI386Glibc23IncludingGTKLib.tar
cd Gabedit
./gabedit
```

6-4 Unpack and install under MacOSX11 using the binary file

download Gabedit207MacOSX.tar.gz file from http://gabedit.sourceforge.net/

Execute the following commands (under X11) :

```
gunzip    Gabedit210MacOSX.tar.gz
tar  -xvf    Gabedit210MacOSX.tar
cd  Gabedit210MacOSX11
./gabedit.sh
```

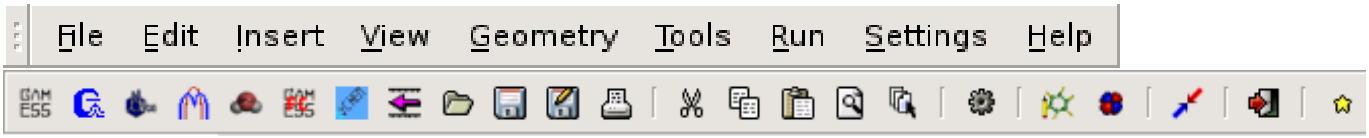
6-5 Unpack and install under Windows system

download setupGabedit210.exe file from http://gabedit.sourceforge.net/

Click to setupGabedit210.exe file.

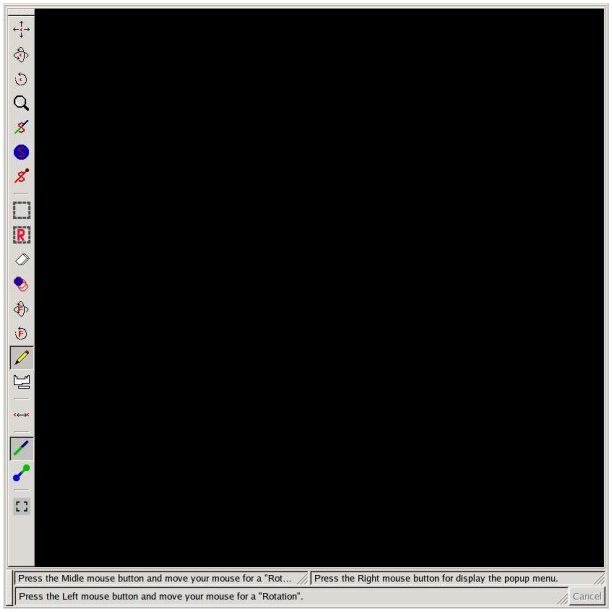
Execute the Gabedit.exe program

7) Detailed instructions for building molecule, creation of input file and submit a job with Gamess-US, Gaussian, Molcas, Molpro, MPQC, PCGamess and Q-Chem



7-1 *Building Molecules*

From the principal menu of Gabedit, select ***Geometry/Draw****. You can also click to 'Draw Geometry' icon (*  *). You will obtain a new window (black by default).*



You can use it to rapidly sketch in molecules and examine them in three dimensions.

For this, Gabedit offers various possibilities :

1) You can **read** the structure of a molecule from a existing file.
   For this using the right button of mouse, click in drawing area (black by default) and select ***Read***.
2) You can build linear molecules, ring molecules, molecules with an axis of symmetry, Polypeptides, Polynucleic acids, nanotubes. For this click on drawing area (with right button of mouse) and select ***Build***.
3) You can also build molecules from atoms or fragments (From ***Add/Your Fragment***).

   About 100 fragments are at disposable in Gabedit. You can also create your personal fragments.
4) You can modify the molecule in 3D. For this,
   First : Select one or some atoms by using  icon for a free selection or  icon for select a fragment of molecule. These 2 icons are in the toolbar window of 'Draw Geometry' window (right-hand side of this window). You can use the Shift key of keyboard to select separated fragments.
   Then :
   - You can move or rotate the selected atoms by using  ,  or  icons.

   Note that you can measure atom-atom distance, angles and torsion angles. For this, click to the  icon and select four atoms of the molecule.

- To delete the selected atoms click to icon and click on one of the selected atoms.

- To add(or replace) an atom click to icon and select the atom to be inserted (by clicking on icon). Then click on drawing area. If you have clicked on an atom, this atom is replaced.

5) You can optimize the structure by a Molecular Mechanics calculation implemented in Gabedit. For this, select Molecular ***Mechanics/Optimization.*** Set your favorite parameters and click to OK button.

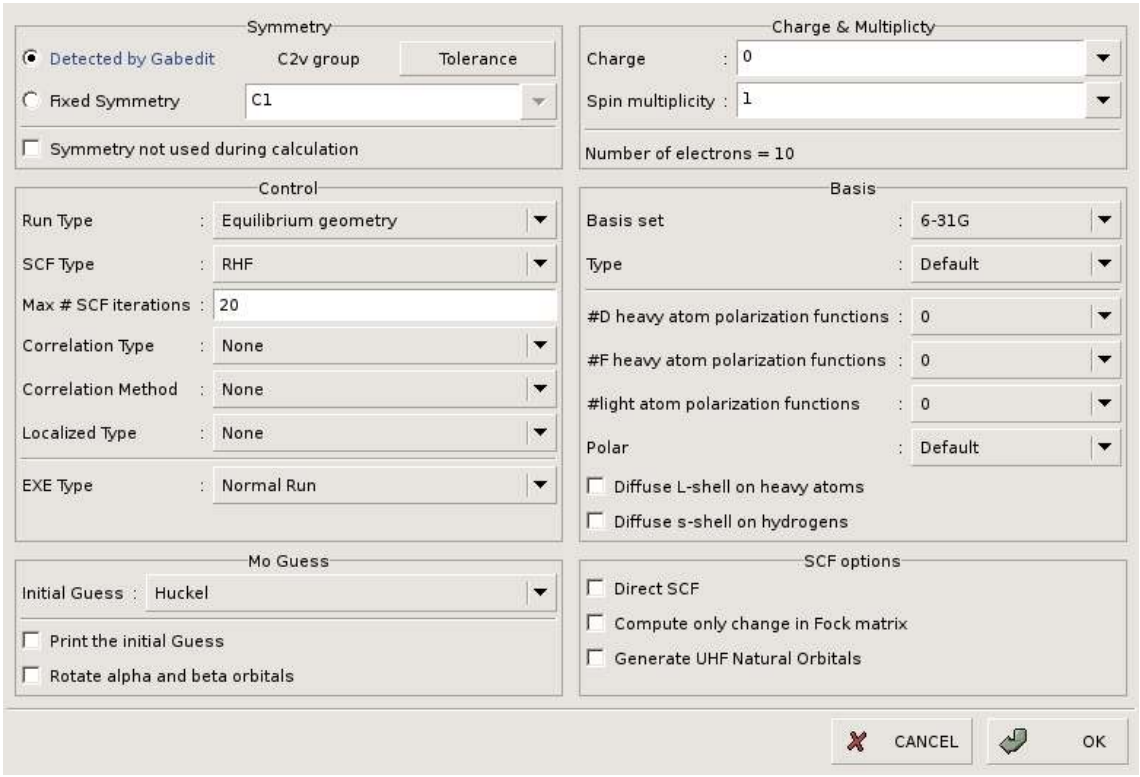
6) You can run a Molecular dynamic simulation by a Molecular Mechanics calculation implemented in Gabedit. For this, select Molecular ***Mechanics/Molecular Dynamics.*** Set your favorite parameters and click to OK button.

7-2 *Creation of an input file for Gamess-US or PCGamess*

Close the geometry window.

On the principal toolbar, Click to Gamess(for Gamess-US or for PCGamess) icon (you can also use the principal menu : ***File/New)***.

You will obtain a new window.



Then, select charge of system and spin multiplicity of your system.
select your method (Run type, SCF Type, Correlation type), basis (BASIS Frame)

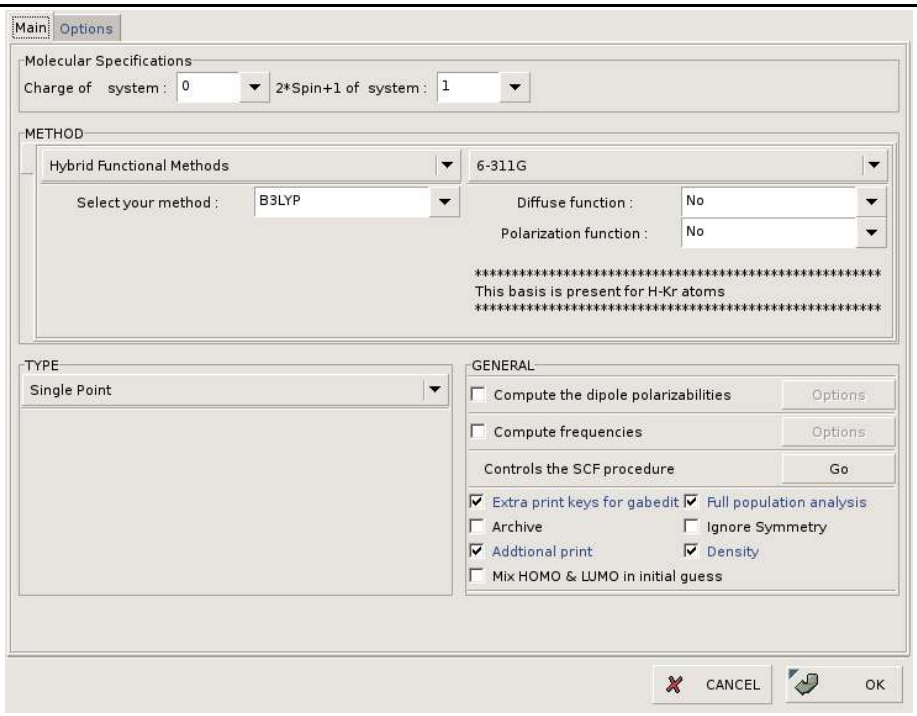
After clicking on the OK button, Gabedit generates the input file and puts this file in a text editor. Your can use the text editor to edit this file.

7-3 *Creation of an input file for Gaussian*

Close the geometry window.

On the principal toolbar, Click to Gaussian( ) icon (you can also use the principal menu : ***File/New/Gaussian Input)***.

You will obtain a new window.



Then, select your method (METHOD Frame), basis (BASIS Frame) and the type of calculation (single point or Geometry optimization) (TYPE Frame).

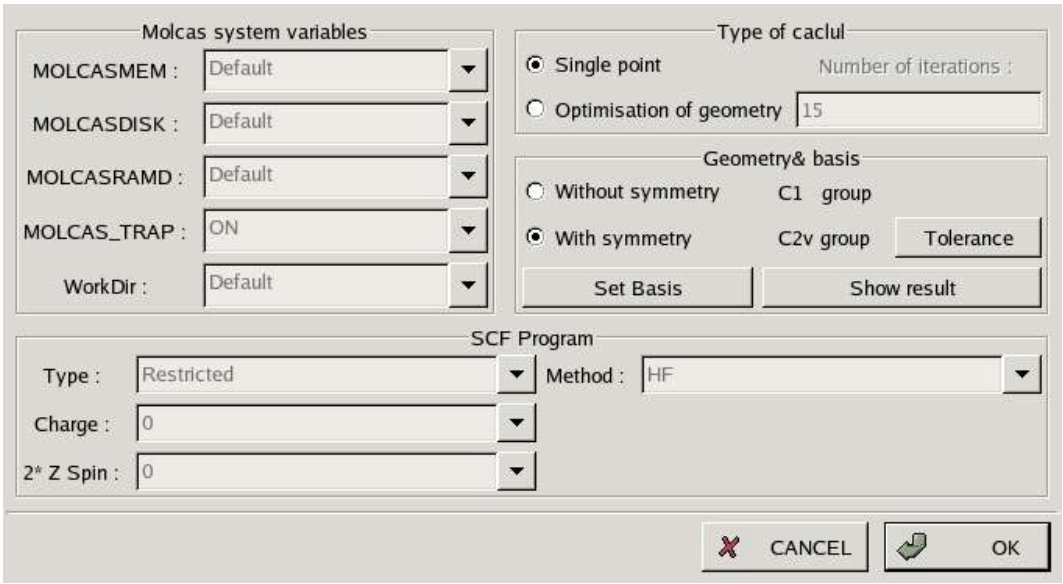
After clicking on the OK button, Gabedit generates the input file and puts this file in a text editor. Your can use the text editor to edit this file.

7-4 *Creation of an input file for Molcas*

Close the geometry window**.**

On the principal toolbar, Click to Molcas( ) icon (you can also use the principal menu : ***File/New/Molcas***).

You will have a new window.

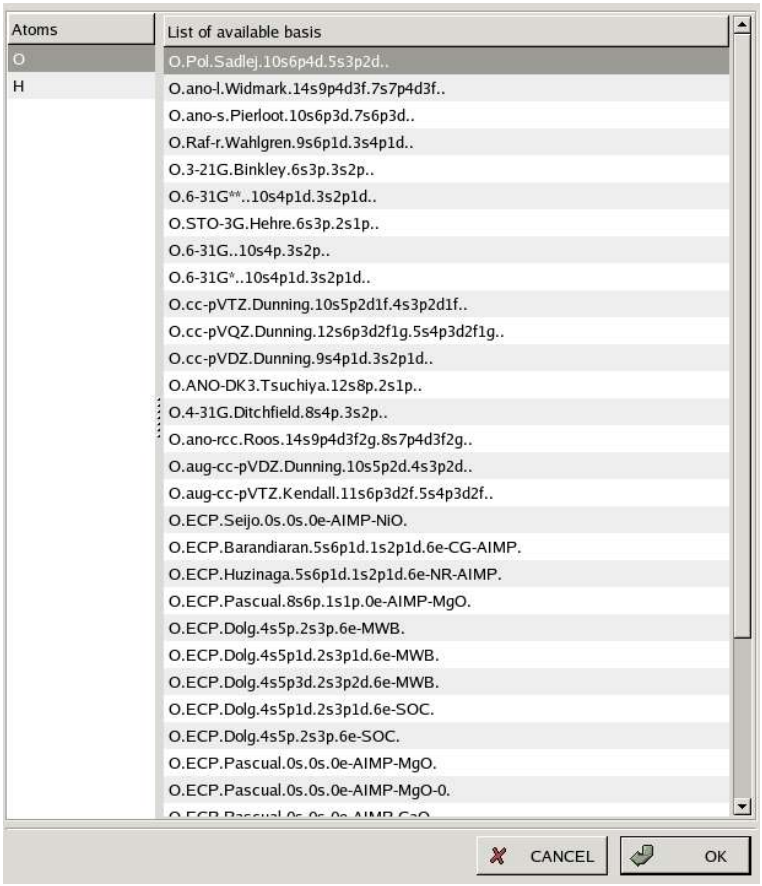


Gabedit detects the symmetry of molecule and the list of atoms to insert in the input file.
Gabedit use default tolerance parameters for compute the symmetry.
By clicking on Tolerance button you can change these parameters.

By default **Gabedit** set the basis to STO3G for all atoms. You can change this basis by clicking on Set Basis button.

Choose the method (from the SCF Program frame).

After clicking on the OK button, Gabedit generates the input file and puts this file in a text editor. Your can use the text editor for editing this file.



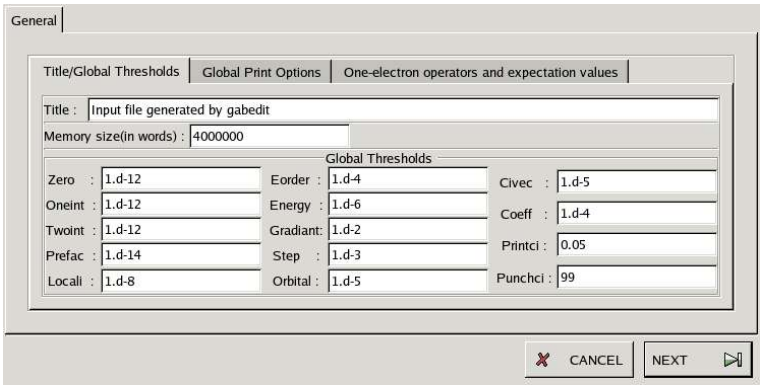
To choose the basis for an atom :
Select the atom from the left list.
Select the basis for the selected atom from the right list.

Finally click to OK button.

7-5 *Creation of an input file for Molpro*

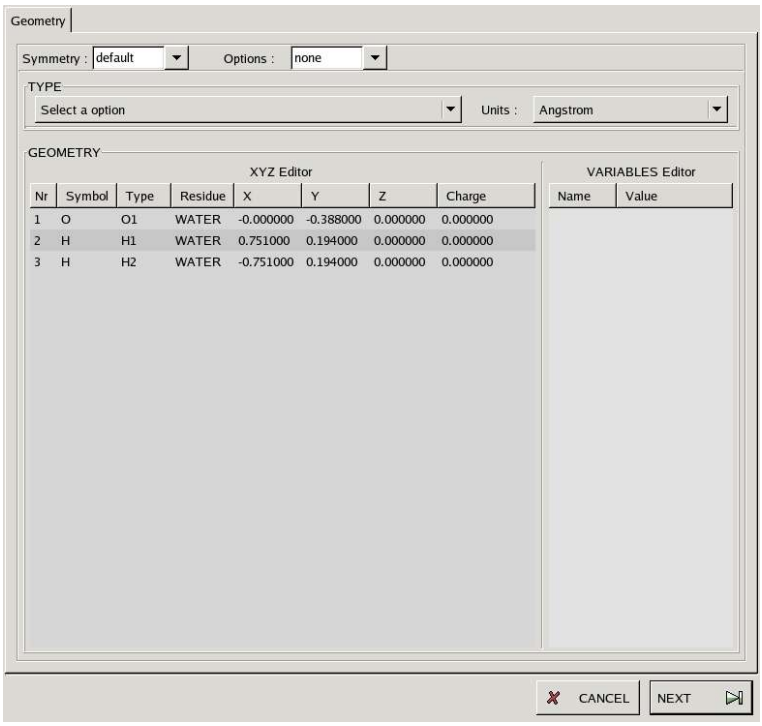
Close the geometry window.

On the principal toolbar, Click to Molpro( ) icon (you can also use the principal menu : ***File/New/Molpro Input***). You will obtain a new window.



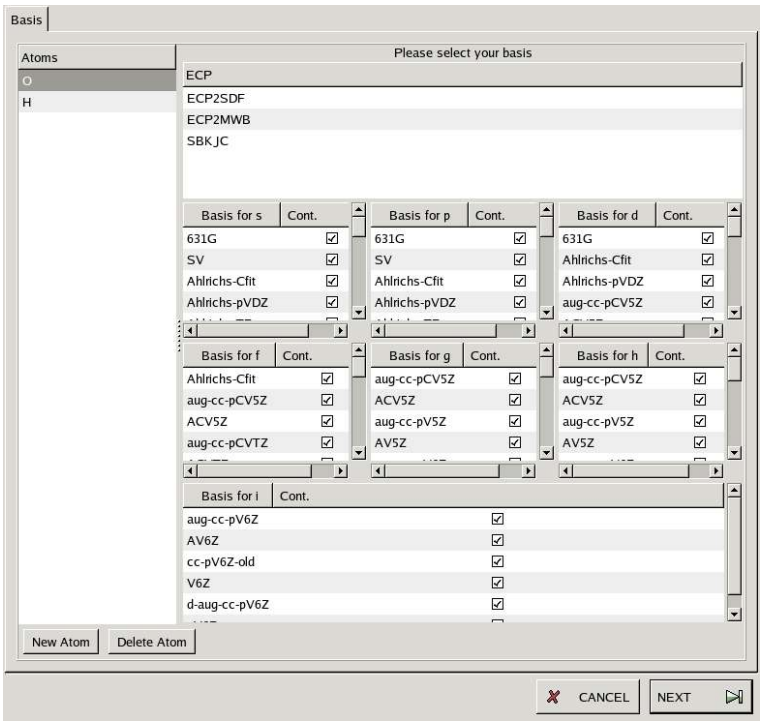
Gabedit sets the general parameters to default values in Molpro. You can change these parameters in this window.
Click to NEXT button.

You will obtain a new window.



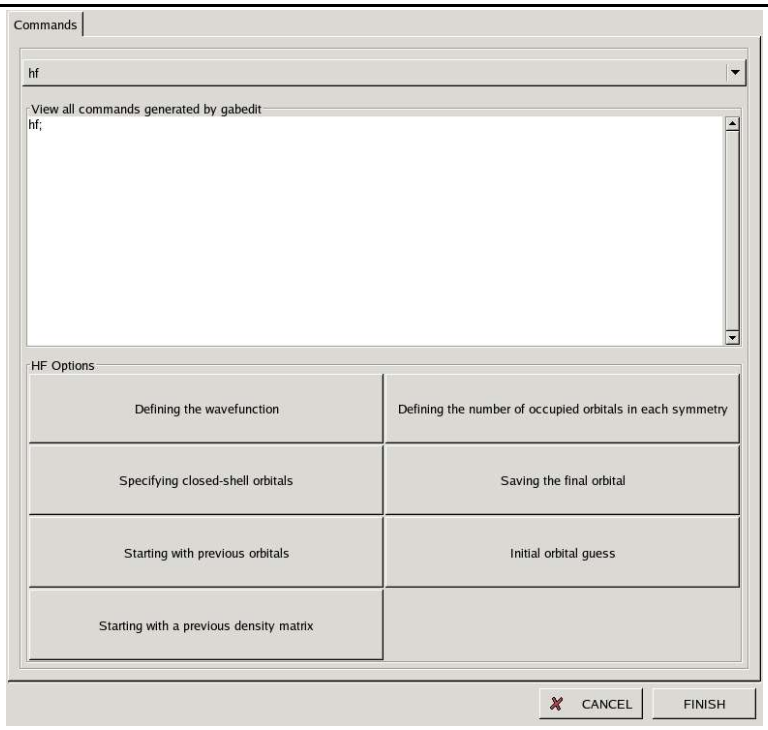
In this window, you obtain the geometry (XYZ or Z-Matrix) of your molecule.
By default no variables coordinates are defined. To define the coordinates (VARIABLES) to optimize for a geometry optimization : Click (with right button of the mouse) on the list of coordinates. To select the are to be changed in the optimization process. (In the example, they are XO5, YO5, ZO5, XO9, YO9, ZO9).
You can also click (right button of mouse) on the list of VARIABLES for render fixed the selected ones.
To modify the coordinates of an atom (or a variable) double click on this atom and modify.
From the pop up menu (right button of mouse) you have also other utilities : sort, multiply by a0 , divide by a0, convert in Z-matrix (or in xyz), draw your geometry...

Click to NEXT button.
You will obtain a new window for choose the basis sets for the various atoms.



To choose the basis for an atom :
- Select the atom from the left list.
- From the right list, Select the ECP and/or the basis for selected atom.

Click to NEXT button.
You will get a new window for choose the calculation methods.



To choose a method click to the list of the methods, available at the top of the window.

To change the default parameters of this method, click to buttons at the bottom of the window.

To add a further method, click to the list of methods (at top of the window).

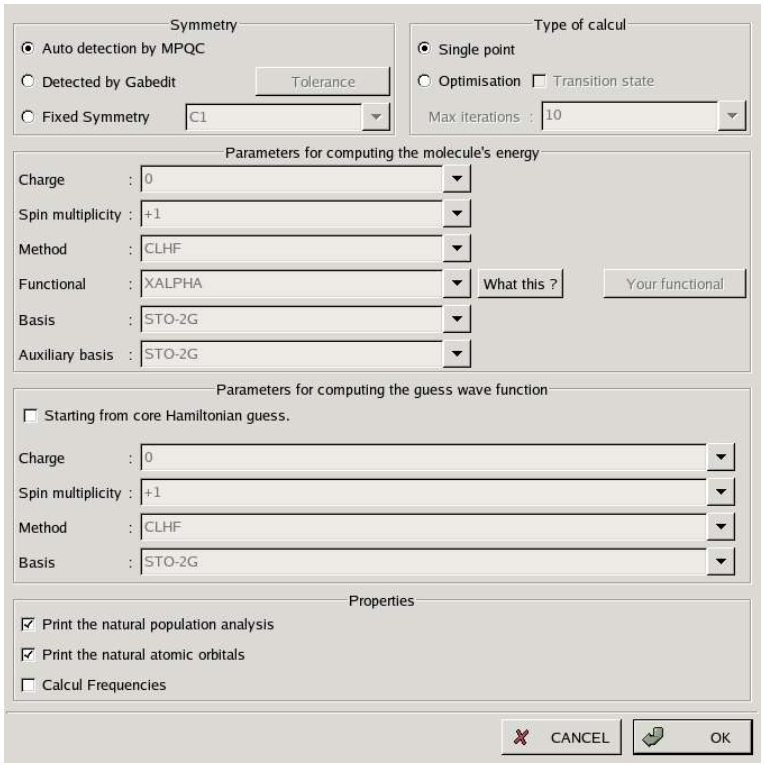
After clicking on the FINISH button, Gabedit generates the input file and puts this file in a text editor. Your can use the text editor for editing this file.

7-6 *Creation of an input file for MPQC*

Close the geometry window**.**

On the principal toolbar, Click to MPQC() icon

You will obtain a new window.



Select the group symmetry.

Select the type of calculation : single point, optimization (local minimum or transition state).

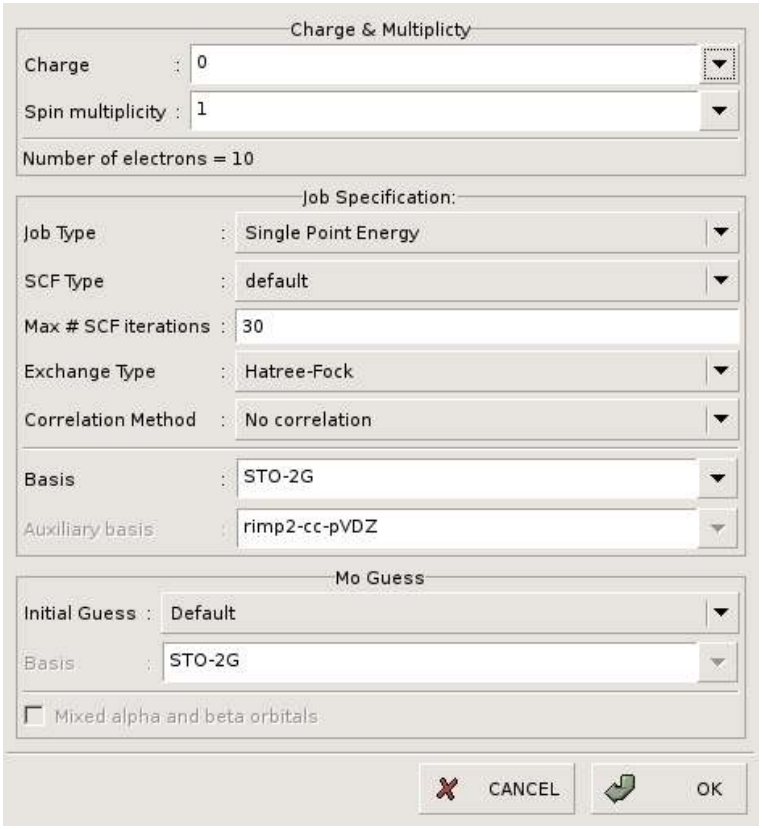
Set the parameters (Charge, multiplicity, method, basis...) used for computing the molecule's energy.
Set the parameters (Charge, multiplicity, method, basis...) used for computing guess wave function.
Select the properties to calculate (atomic natural orbitals, natural populations, frequencies).

After clicking on the OK button, Gabedit generates the input file and puts this file in a text editor.
Your can use the text editor for editing this file.

7-7 *Creation of an input file for Q-Chem*

Close the geometry window**.**

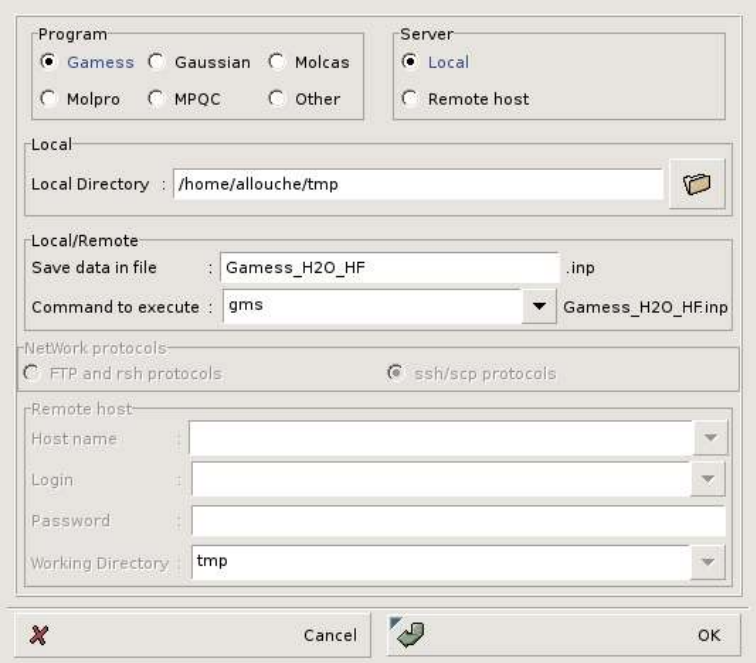
On the principal toolbar, Click to Q-Chem( ) icon. You will obtain a new window.



Set the parameters.
After clicking on the OK button, Gabedit generates the input file and puts this file in a text editor.
Your can use the text editor for editing this file.

7-8 ***Submit a job.***

Click to run ( ) icon. You will get a new window.



- Set the directory (*Local Directory :*).

- Set the name of the input file (*Save data in file :*)

click to OK button for submit your job.

A) Command for submit a job

Gabedit set this command to 'gms', 'nohup g98', 'nohup molcas' , 'nohup molpro' and 'nohup mpqc' for Gamess-US, Gaussian, Molcas, Molpro and MPQC respectively. However you can modify the default value from **Settings/Preferences** of the principal menu of Gabedit.

Under Windows :

If you want to use winGamess, you shoud set the winGamess directory from Settings/Preferences.
If you want to use PCGamess, you shoud set the PCGamess directory from Settings/Preferences.
For run Gamess-US the default command is gamess.05.exe. If you version of Gamess-US is not 05, you should replace 05 by the number version of your Gamess version.

Under Unix (Linux or MacOS X11) :

if you want to use Gamess-US, you should change the 'gms' and 'rungms' scripts of Gamess-US :
In 'gms' file : replace line './rungms $JOB $VERNO $NNODES >& $LOGFILE' by the 2 lines :

```
set GAMESS_INSTALL_DIR=`dirname $0`
 $GAMESS_INSTALL_DIR/rungms $JOB $VERNO $NNODES >& $LOGFILE
```

In 'rungms' file replace set GMSPATH=./ by

```
set GMSPATH=`dirname $0`
```

You can also use any command with any number of parameters but the last parameter should be the name of the input file. In Gabedit/utils directory, you have several examples for run Gamess-Us, Gaussian, Molcas, Molpro and MPQC using a batch system (PBD, LSF or LoadLeveler batch system). You should be install the shell command on your remote server. Edit the shell file and set the correct value of parameters which correspond to your Gamess-US, Gaussian, Molcas, Molpro or MPQC installation.

B) Submit a job on a remote server

You can submit your job on your local machine (only on Linux and unix systems) or on a remote

server. For Windows system, you can not run Gaussian, Molcas, Molpro and MPQC on your local machine. You should submit your job on a remote (Linux or Unix) server.

For submit your job on a remote server, you should configure Gabedit to obtain the default network protocol (rsh or ssh). For this, select ***Settings/Preferences*** of the principal menu of Gabedit and click to '***Other***' Window. Then select your favourite protocol. Select also your favourite Batch system.

*** For windows system :***

- *you should select the program pscp and plink (these 2 programs are in Gabedit installation directory).*
- *You should execute putty program (once is enough)*, for add your server on the list of authorized servers.

*** For linux(and unix) system** : click to Help button for obtain all the informations about the configuration of your system, configuration required for being able to submit a job on a remote server.*

After submitting your job, you can show the list of your jobs on the remote server (and kill a job if necessary). For this, select ***Tools/Batch/Remote/User*** from the principal menu of Gabedit.

7-9 Visualizing the Results

Select the notebook of the output file.

- Click to ***Update/end*** button, if your job is submitted on the local machine.

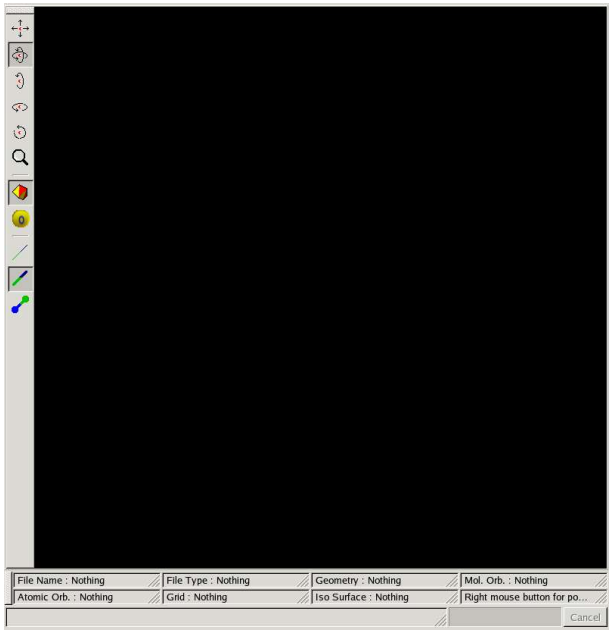
- Click to ***Get All*** files button, if your job is submitted on a remote machine.

- You can visualize the geometry convergence by clicking on the ***Geom. Conv***. Button.

- Click to ***Dens. Orb*** button, for visualize the orbitals, the electronic density, electric dipole or the vibration.

Visualizing orbitals, density or other :

After clicking on the ***Dens. Orb***. button (or on the  icon from the principal toolbar of Gabedit), you will obtain a new window.



- You can read orbitals from a : Gaussian output file, Molpro output file, Gabedit file or Molden file. For this using the right button of mouse, click in drawing area (black by default) and select ***Orbitals*** from the pop up menu. Choose a type of file and the the file.

After reading the orbitals, you can select (you will have a window with the list of all orbitals) an orbital. You can also calculate the electronic density using these orbitals (Density/Electronic from the pop up menu).

For choose the isovalue, select ***Surfaces/resetisovalue*** from the pop up menu.
For create a new surface select ***Surfaces/new surface*** from the pop up menu.
For delete all surfaces select ***Surfaces/Delete All*** from the pop up menu.
For choose the type of surface, select ***Render/Surface*** from the pop up menu.
You can use the rotation ( , ), zoom () and perspective ()icons. Then by moving the mouse while holding down the left button you can obtain an optimal image.
You can also obtain an optimal image by clicking on "O" button.
You can also obtain an optimal image by setting the camera parameters. For this select ***Set/Camera*** from the pop up menu.
Finally, you can create a povray file by selecting ***Export/Povray*** from the pop up menu.
Finally, you can save the image on a BMP, PPM, JPEG, PNG, or PS file by selecting ***Screen Capture*** from the pop up menu.

- You can also read orbitals, density, electrostatic potential, laplacian from a cube file.

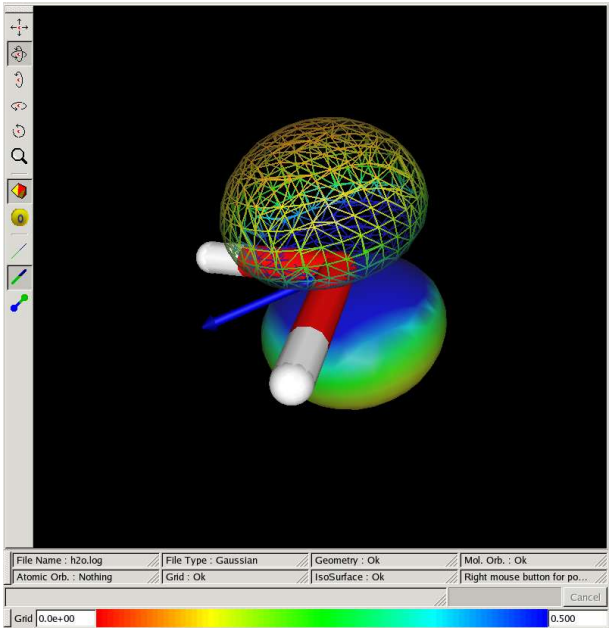
The cube format file supported by Gabedit are : Gaussian cube file (orbitals, density, potential, laplacian), Molpro cube file(orbitals, density, potential, laplacian), Gabedit cube file (see the last page of the manual), ADF tape 41 (orbitals and density), M2MSI (ASCII format from Molcas software).

For read a cube file, select ***Cube*** from the pop up menu, the choose the format file.

With Gabedit you can also subtract grid data from a file from the currently loaded data by selecting ***Cube/Subtract*** from the pop up menu.

- With Gabedit you can also create an isosurface colorcoded with another grid. For this :
  - read (or create from orbitals) the grid used to color the surface.
  - Save this grid in Gabedit cube file.
  - read (or create from orbitals) the grid colorcoded by the old grid.
  - Form the pop up menu, select ***Cube/Color Mapping*** and read the Gabedit cube file.

- At the bottom of the Drawing window, set the min and the max values used to color the surface.



What this ? Water molecule, HOMO orbital colorcoded with the electronic density. Isovalue = 0.1

Visualizing of dipole, xyz axes and the principal axes of molecule.

Gabedit read orbitals, geometry and dipole from the output file of Gaussian and Molpro.
However you can set the x, y and z components of dipole. For this from the pop up menu select ***Set/Dipole*** and set your values. You can also change the color used for draw the dipole.
You can also compute the dipole, numerically, from the electronic density :
Set/Compute Dipole from density.

To show xyz axes, select ***Render/Show XYZ axes*** (from the pop up menu).
To change the color used for draw these axes, select ***Set/XYZ axes properties.***

To show the principal axes, select ***Render/Show the principal axes*** (from the pop up menu).
To change the color used for draw these axes, select ***Set/ the principal axes properties.***

Animation of vibration :

From the pop up menu select ***Animation/Vibration***. You will obtain a new window.

1) From the menu of this window (or from the pop up menu of this window obtain by clicking(right button of mouse) on the list of frequencies), choose the type of file to read.

With Gabedit you can read frequencies and the normal modes from:
- a Gaussian output file
- a Molpro ouput file
- an ADF(version 2004) output file
- a Gabedit file
- a Molden file

2) Select a frequency from the list.

3) Set the value of ***Scale factor***, ***Time step***, ***Arrow radius*** and ***Steps by cycle*** parameters (if necessary).

3) By rotation and zoom find the optimal image.

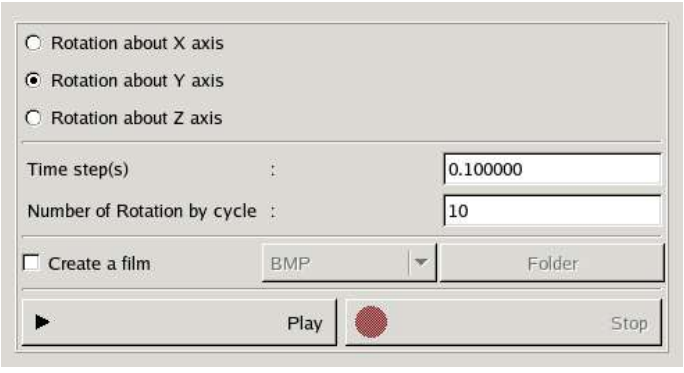
4) Click to **Play** button for animate the vibration.

5) Click to **Stop** button for stop the animation.

6) For create a animated file, select **Create a series of BMP images** and click to **Play** button. After one cycle you can stop the animation. Using convert program, you can create a MNG or a GIF animated file from the BMP files generated by Gabedit.

Animation of rotation :

From the pop up menu select ***Animation/Rotation***. You will obtain a new window.



Choose the axis of rotation.
By rotation and zoom, find the optimal image.

Click to **Play** button for animate the rotation.

You can also create an animated file for this animation (see the vibration animation section).

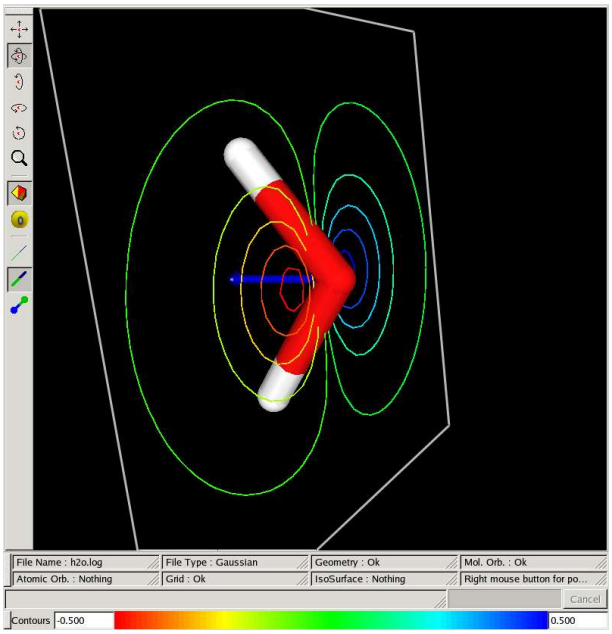
Animation of geometry convergence :

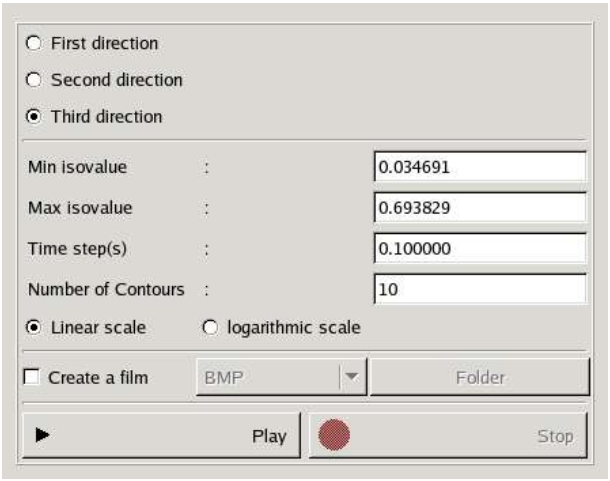
From the pop up menu select ***Animation/geometry convergence***.
You will obtain a new window.

By rotation and zoom, find the optimal image.
Click to **Play** button for start animation.
You can also create an animated file for this animation (see the vibration animation section).

Animation of contours :

From the pop up menu select ***Animation/Contours***
You will obtain a new window.

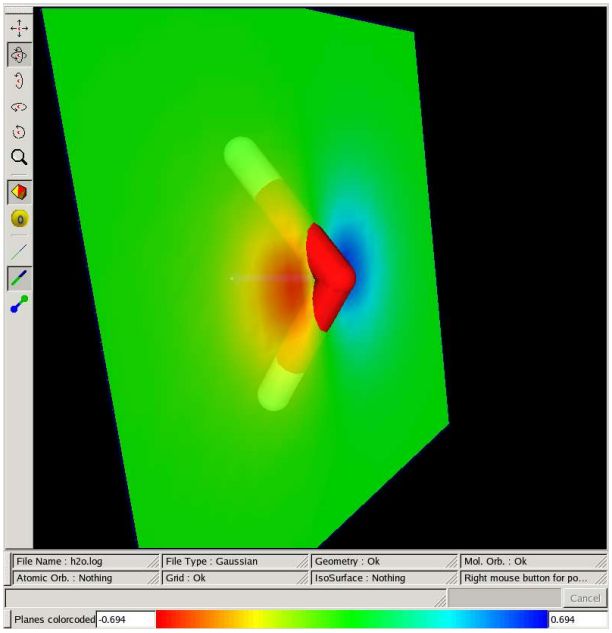


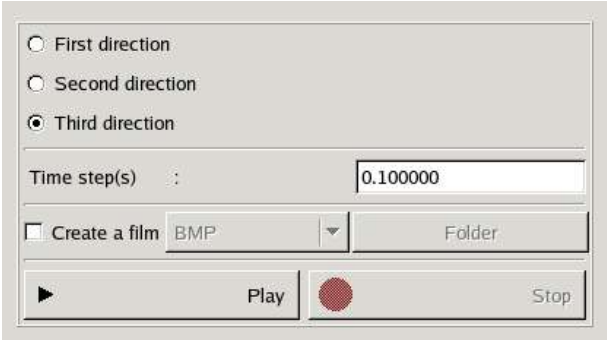


By rotation and zoom, find the optimal image.
Select the direction, min isovalue, max isovalue, and the number of contours in each plane.
Set the min and the max value used for create the colormap (On the bottom of the left window).
Click to **Play** button for start animation.
You can also create an animated file for this animation (see the vibration animation section).

Animation of planes colorcoded :

From the pop up menu select ***Animation/Planes colorcoded*** You will obtain a new window.





By rotation and zoom, find the optimal image.
Set the min and the max value used for create the colormap (On the bottom of the left window).
Click to **Play** button for start animation.
You can also create an animated file for this animation (see the vibration animation section).

8) The Gabedit Format (.gab)

Gabedit can support any other programs via the Gabedit format.

Not all of the below sections are required, you could have

{[Atoms],[Basis] and [MO]} , here [AO] is optional (this is used for calculate the difference between the electronic density of molecule and the electronic density of atoms).

Or { [GEOCONV] with [GEOMETRIES]},

Or { [FREQ],[FR-COORD],[FR-NORM-COORD], here [INT] is optional}

First Line:

[Gabedit Format] (Sphe | Cart)

The workings are with Spherical or Cartesian Gaussian Basis format, indicated by the Sphe or Cart keyword.

Coordinates of Atoms for the Electron Density/Molecular orbitals:

```
[Atoms] (Angs|AU)
element_name number atomic_number x y z
...
```

The workings are with Angstroms or Atomic Units, indicated by the Angs or AU keyword.

Specification of the basis-set consisting of contracted Gaussian Type Orbitals.

[Basis]
atom_sequence_number1 0
shell_label number_of_primitives 1.00
exponent_primitive_1 contraction_coefficient_1 (contraction_coefficient_1)
...
empty line
atom_sequence__number2 0
shell_label number_of_primitives 1.00
exponent_primitive_1 contraction_coefficient_1 (contraction_coefficient_1)
...
empty line
recognized shell_labels:

's','p','d','f','g','h','i','j','k','sp', 'sd', ...

For 'sp', 'sd'... shells two contraction coefficients must be given, for both first and second functions.

All workings with the **[Basis]** keyword are in Atomic Units.

Specification of the molecular orbitals.

The molecular orbitals and their occupation number are specified in the **[MO]** section. From this information a density matrix can be constructed.

```
[MO]
Sym= symmetry_label_1
Ene= mo_energy_1
Spin= (Alpha|Beta)
Occup= mo_occupation_number_1
ao_number_1 mo_coefficient_1
...
ao_number_n mo_coefficient_n
....
```

```
Sym= symmetry_label_N
Ene= mo_energy_N
Spin= (Alpha|Beta)
Occup= mo_occupation_number_N
ao_number_1 mo_coefficient_1
...
ao_number_n mo_coefficient_n
```

Specification of the atomic orbitals.

The atomic orbitals and their occupation number are specified in the **[AO]** section.

[AO]
Atom= Atomic Symbol_1
Sym= symmetry_label_1
Ene= ao_energy_1
Spin= (Alpha|Beta)
Occup= ao_occupation_number_1
ao_number_1 ao_coefficient_1
...
ao_number_n ao_coefficient_n
....
Atom= Atomic Symbol_i
Sym= symmetry_label_N
Ene= ao_energy_N
Spin= (Alpha|Beta)
Occup= ao_occupation_number_N
ao_number_1 ao_coefficient_1
...
ao_number_n ao_coefficient_n

Specification of frequencies and corresponding normal coordinates.

The atomic coordinates x,y,z and atomic displacements dx,dy,dz are all in Bohr (Atomic Unit of length).

[FREQ]
frequency_1
...
frequency_n
[FR-COORD]
atom_1_element_string x y z
...
atom_n_element_string x y z
[FR-NORM-COORD]
vibration vibration_number_1
atom_1_dx atom_1_dy atom_1_dz
...
atom_n_dx atom_n_dy atom_n_dz
....
vibration vibration_number_N
atom_1_dx atom_1_dy atom_1_dz
...
atom_n_dx atom_n_dy atom_n_dz
[INT]
ir_intensity_1 raman_intensity_1
...

ir_intensity_n raman_intensity_n

The Geometry Convergence section

The max-force, rms-force, max-step and rms-step sections are optional.
The atomic coordinates x,y,z are in angstroms unit.

[GEOCONV]
energy
geometry1_energy
...
geometryn_energy
max-force
geometry_1_maximum_force
...
geometry_n_maximum_force
rms-force
geometry_1_rms_force
...
geometry_n_rms_force
max-step
geometry_1_maximum_step
...
geometry_n_maximum_step
rms-step
geometry_1_rms_step
...
geometry_n_rms_step

[GEOMETRIES]
Number_of_atoms
title or empty line (Geometry number 1)
atom_1_element_string x y z
...
atom_(Number_of_atoms)_element_string x y z
...
...
...
Number_of_atoms
title or empty line (Geometry number n)
atom_1_element_string x y z
...
atom_(Number_of_atoms)_element_string x y z

The Molecular Dynamics section

Coord in Ang, Velocity in AKMA, time in fs, Energy in Kcal/mol. residuNumber=0,1,2....

[MD]

number_of_geometries

nAtoms time(fs) TotalEnery KineticEnergy PotentialEnergy

Symbol_1 X_1 Y_1 Z_1 VX_1 VY_1 VZ_1 Charge AmberType PDBType ResiduName ResiduNumber

.....

Symbol_n X_n Y_n Z_n VX_n VY_n VZ_n Charge AmberType PDBType ResiduName ResiduNumber

.....

.....

.....

nAtoms time(fs) TotalEnery KineticEnergy PotentialEnergy

Symbol_1 X_1 Y_1 Z_1 VX_1 VY_1 VZ_1 Charge AmberType PDBType ResiduName ResiduNumber

.....

Symbol_n X_n Y_n Z_n VX_n VY_n VZ_n Charge AmberType PDBType ResiduName ResiduNumber

Finally, in the Gabedit/utils/examples directory you have 3 examples files with Gabedit format.

These 3 files are also available on the Gabedit home page :

http://gabedit.sourceforge.net/Examples/exampleCartezian.gab

http://gabedit.sourceforge.net/Examples/exampleSpheric.gab

http://gabedit.sourceforge.net/Examples/exampleGeoConv.gab

9) The Gabedit cube format (.gcube)

The first line is a comment

The second line is a comment

numberOfAtoms X-Origin Y-Origin Z-Origin
N1 X1 Y1 Z1 *# number of points, X, Y and Z of increments in the slowest running direction*
N2 X2 Y2 Z2
N3 X3 Y3 Z3 *# number of points, X, Y and Z of increments in the fastest running direction*
Z1 Chg1 X1, Y1, Z1 *# Atomic number (integer), charge(real), and coordinates for each atom*
....
....

(N1*N2) records (length N3) v*alues of the density at each point in the grid. E*ach row contain 6 reals separated by a black space. If N_3 is not a multiple of six, then there may be blank space in some lines.

A example of a Gabedit cube file :

Grid file generated by Gabedit
Density
3 -4.000000 -4.000000 -4.000000
40 0.205128 0.000000 0.000000
40 0.000000 0.205128 0.000000
40 0.000000 0.000000 0.205128
8 0.000000 0.000000 0.000000 0.256576
1 0.000000 0.000000 1.456833 -1.026304
1 0.000000 0.000000 -1.456833 -1.026304
-0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000
-0.000000 -0.000000 -0.000000 -0.000000 -0.000001 -0.000001
-0.000001 -0.000001 -0.000002 -0.000002 -0.000002 -0.000003
-0.000003 -0.000003 -0.000003 -0.000003 -0.000003 -0.000003

-0.000003 -0.000003 -0.000002 -0.000002 -0.000001 -0.000001
-0.000001 -0.000001 -0.000000 -0.000000 -0.000000 -0.000000
-0.000000 -0.000000 -0.000000 -0.000000
-0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000
-0.000000 -0.000000 -0.000000 -0.000001 -0.000001 -0.000001
-0.000002 -0.000002 -0.000003 -0.000004 -0.000004 -0.000005
-0.000006 -0.000006 -0.000006 -0.000006 -0.000006 -0.000006
.....

10) Tutorial

A tutorial for Gabedit is available on the Gabedit home page :

http://gabedit.sourceforge.net/tutorial.html