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Documentations

(See also Journal of Computational Chemistry, 32 (2011) 174–182. DOI: 10.1002/jcc.21600)

What is Gabedit ?

Gabedit is a graphical user interface to computational chemistry packages like Gamess-US, Gaussian, Molcas, Molpro, MPQC, NWChem, OpenMopac, Orca, 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.

Contents

Major features

- Gabedit can creates input file for GAMESS(US), GAUSSIAN, MOLCAS, MOLPRO , MPQC, NWChem, OpenMopac, Orca, PCGamess and Q-Chem.
- Gabedit can graphically display a variety of Gamess-US, Gaussian, Molcas, Molpro, MPQC, NWChem, OpenMopac, Orca, 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, Raman, ECD, NMR computed spectra.
- Gabedit can generate a povray file for geometry (including hydrogen's bond),surfaces (including colorcoded surfaces), contours, planes colorcoded.
- Gabedit can export picture in EPS, PS, PDF and svg files.
- 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).

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.

Availability

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

Citation

Please use the following citations in any report or publication :
A.R. ALLOUCHE, Gabedit - A graphical user interface for computational chemistry softwares, Journal of Computational Chemistry, 2010, DOI: 10.1002/jcc.21600

License

Installation

Requirements
OpenGL (or Mesa3D) and gtk+.2.4.x (or higher) libraries for UNIX.
Nothing for Linux and Windows systems.

Unpack and install under Linux (and UNIX) system using the source files
download GabeditSrcxxx.tar.gz file from http://gabedit.sourceforge.net/
Execute the following commands:
gunzip GabeditSrcxxx.tar.gz (xxx is the version number of Gabedit)
tar -xvf GabeditSrcxxx.tar
cd GabeditSrcxxx
make
./gabedit

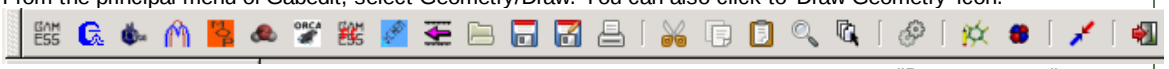
Unpack and install under Linux system using the binary files
Gtk2+ is installed in your system
download GabeditxxxLinuxI386Glibc23.gz from http://gabedit.sourceforge.net/
Execute the following commands:
gunzip GabeditxxxLinuxI386Glibc23.gz
cp GabeditxxxLinuxI386Glibc23 gabedit
chmod u+x gabedit
./gabedit
Gtk2+ is not installed in your system
download setupGabeditxxxwGTK.sh
Execute the following commands:
chmod u+x setupGabeditxxxwGTK.sh
./setupGabeditxxxwGTK.sh

Unpack and install under MacOSX11 using the source files
Download GabeditSrcxxx.tar.gz file from http://gabedit.sourceforge.net/
Install X11 if this is not already installed on your mac (see http://guide.macports.org/#installing.x11)
Install macports (http://www.macports.org/)
Install gtk2 (not gtk) using macports : port install gtk2 (see http://guide.macports.org)
Execute the following commands:
cp platforms/CONFIG.MacPorts CONFIG
make

Unpack and install under Windows system
download setupGabeditxxx.exe file from http://gabedit.sourceforge.net/
Click to setupGabeditxxx.exe file.

Building molecule

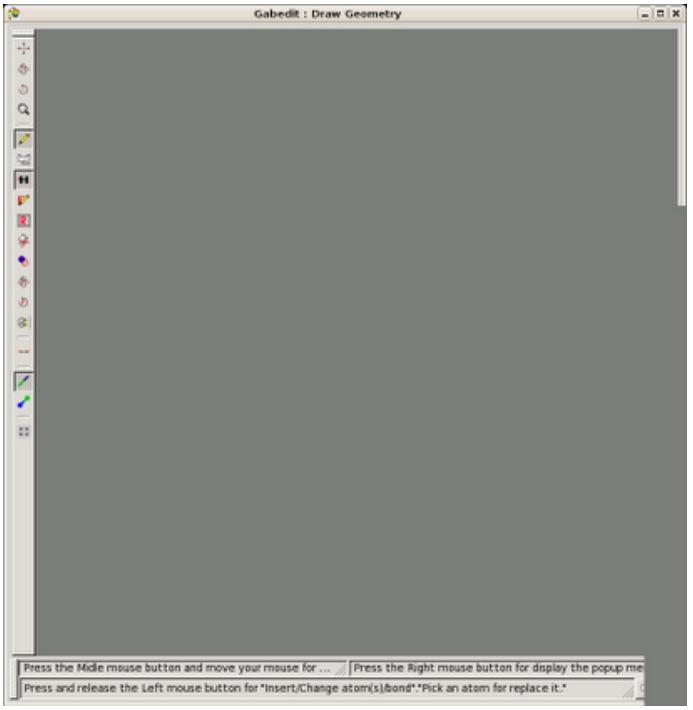
From the principal menu of Gabedit, select Geometry/Draw. You can also click to 'Draw Geometry' icon.



"Draw geometry"

You will obtain a new window (black by default).
You can use it to rapidly sketch in molecules and examine them in three dimensions.You can use it to rapidly sketch

in molecules and examine them in three dimensions.



For this, Gabedit offers various possibilities :

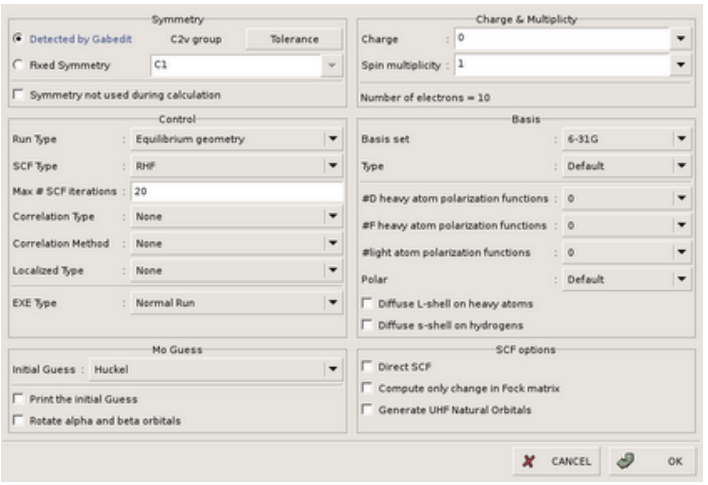
1. You can **read** the structure of a molecule from a existing file.
   For this using the right button of mouse, click in drawing area (black by default) and select ***Read***.
2. You can build linear molecules, ring molecules, molecules with an axis of symmetry, Polypeptides, Polynucleic acids, nanotubes. 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***).
   About 200 fragments are disposable in Gabedit. You can also create your personal fragments.
4. You can modify the molecule in 3D. For this,
   - Select one or some atoms by using
   
   icon. You can use the Shift key of keyboard to select separated fragments.
   - 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. If you have clicked on a bond, this bond is deleted.
   - To add(or replace) an atom click to  icon and select the atom to be inserted (You can change it by clicking on  icon). Then click on drawing area. If you have clicked on an atom, this atom is replaced. Using this icon you can add a bond : click and move your mouse.
5. You can freeze one or more atoms during optimization procedure by a CCP. After selection of atoms to freezing, from menu select "Set/Set selected atoms to freezing during geometry optimization".
6. 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.
7. 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.
8. You can optimize the structure, interactively, using Open Mopac, PCGamess or Orca program. For this, select Semi-Emperical***/"Method".***
9. A Molecular dynamics conformational search is implemented using a MM (Amber 99) or a Semi-Empirical potential . During the production stage Gabedit selects a number geometries. At the end of the molecular dynamic simulation, each selected geometry is optimized. Finaly the geometries are sorted by energy and saved in a file. The very similar geometries can be removed by Gabedit. Gabedit can also optimize these geometries, interactively, using Mopac or PCGamess. Gabedit can also creates input files for Mopac, PCGamess or Gaussian for a post processing.

Creation of input file for a CCP package

Close the geometry window.


"Gamess" "PCGamess" icons

On the principal toolbar, Click to the icon of you favorite CCP (Gamess-US, Gaussian, Molcas, ...). You can also use the principal menu : File/New).
You will obtain a new window.

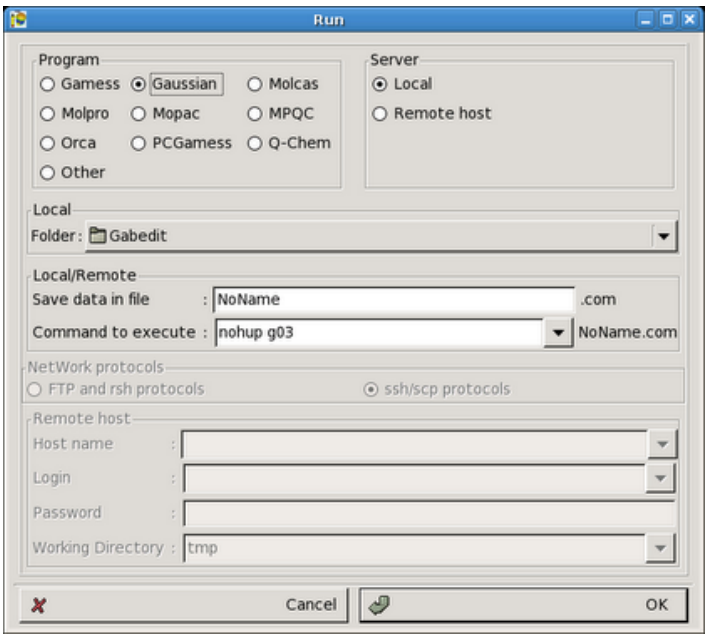


Then, select charge of system and spin multiplicity of your system, you method, the type of calculation....
After clicking on the **OK** button, Gabedit generates the input file and puts this file in a text editor.
Your can use the text editor to edit this file.

Submit a job

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 'submitGMS', '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, the gamess directory should be in your path.

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.

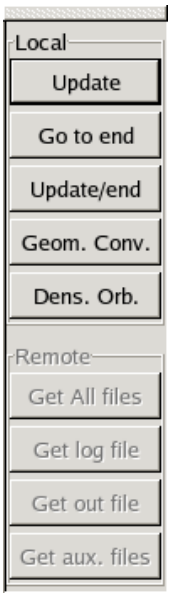
B) Submit a job on a remote server

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.

Visualizing the Results



Select the notebook of the output file.

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

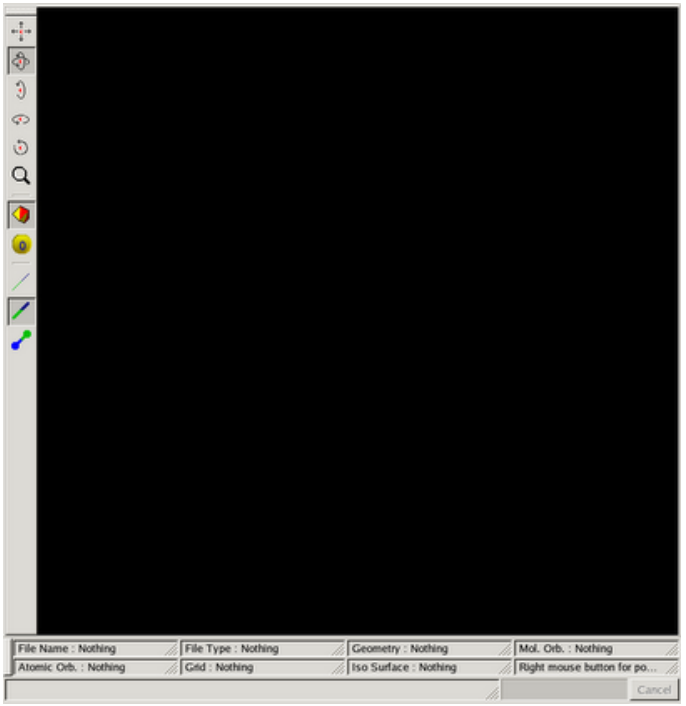
- Click to Get All files button, if your job is submitted on a remote machine.

- 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 :

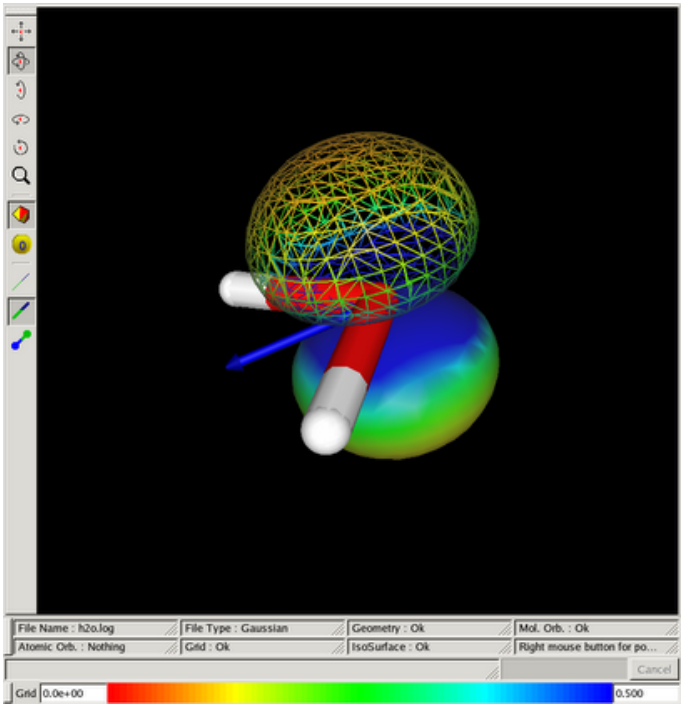
"Dens. Orb."
After clicking on the Dens. Orb. icon (from the principal toolbar of Gabedit), you will obtain a new window.



- You can read orbitals from a : Gamess, Gaussian, Molpro, PCGamess, Q-Chem output file, NWChem, OpenMopac aux 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.

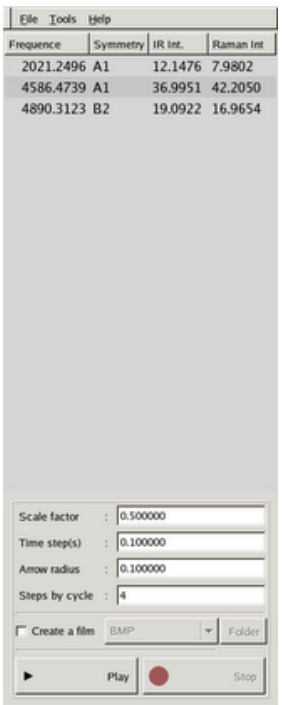
- With Gabedit you can also create an isosurface colorcoded with another grid. For this :
Read (or create from orbitals) the grid used to color the surface.
Save this grid in Gabedit cube file.
Read (or create from orbitals) the grid colorcoded by the old grid.
Form the pop up menu, select Cube/Color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

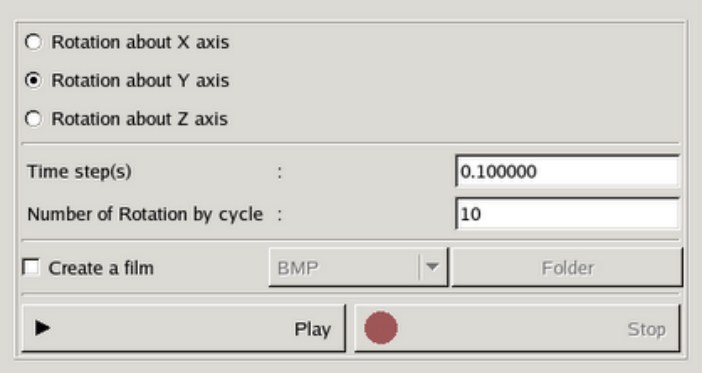
Visualizing of dipole, xyz axes and the principal axes of molecule.
Gabedit read dipole from CCP output file.
However you can set the x, y and z components of dipole. For this from the pop up menu select Set/Dipole and set your values. You can also change the color used for draw the dipole.
You can also 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.



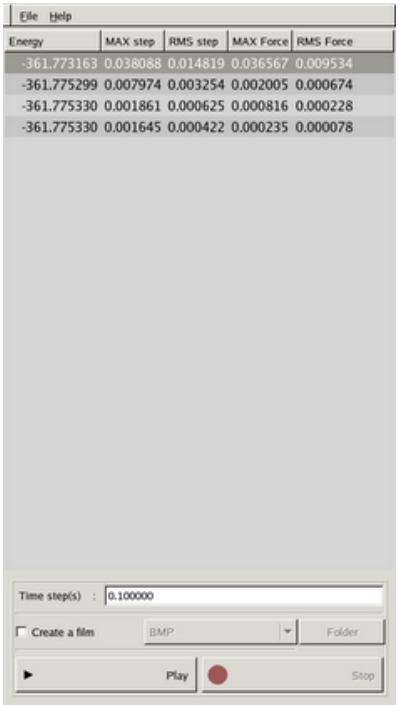
1) From the menu of this window (or from the pop up menu of this window obtain by clicking(right button of mouse) on the list of frequencies), choose the type of file to read.
With Gabedit you can read frequencies and the normal modes from:
- a Gaussian output file
- a Molpro ouput file
- an ADF(version 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.



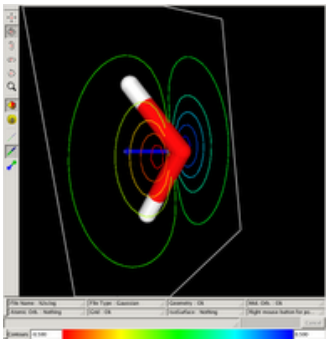
Choose the axis of rotation.
By rotation and zoom, find the optimal image.
Click to Play button for animate the rotation.
You can also create an animated file for this animation (see the vibration animation section).

Animation of geometry convergence :
From the pop up menu select Animation/geometry convergence.

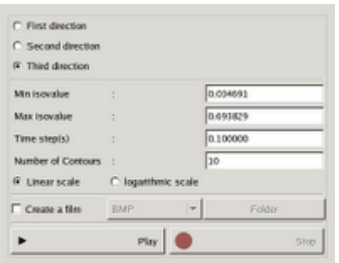


You will obtain a new window.
By rotation and zoom, find the optimal image.
Click to Play button for start animation.
You can also create an animated file for this animation (see the vibration animation section).

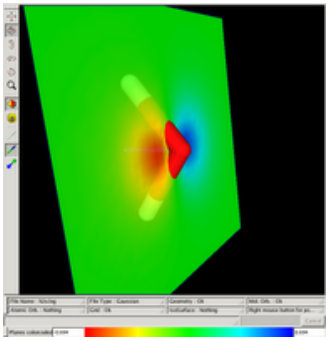
Animation of contours :
From the pop up menu select Animation/Contours
You will obtain a new window.



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.

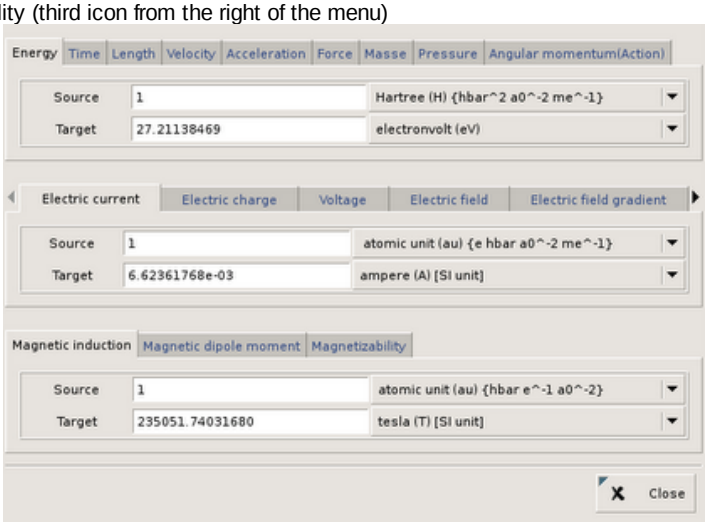


By rotation and zoom, find the optimal image.
Set the min and the max value used for create the colormap (On the bottom of the left window).
Click to Play button for start animation.
You can also create an animated file for this animation (see the vibration animation section).

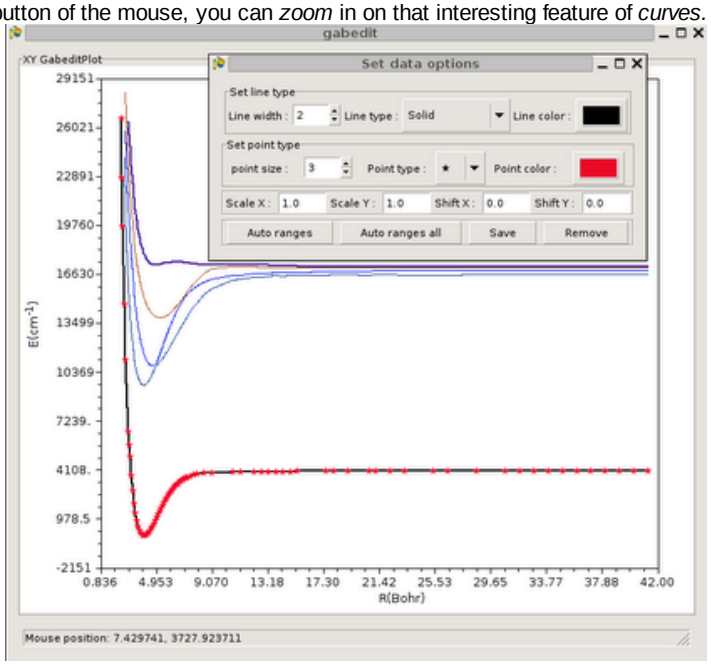
Tools

Several tools are implemented in Gabedit. Gabedit include, among others :

- Unit conversion utility (third icon from the right of the menu)

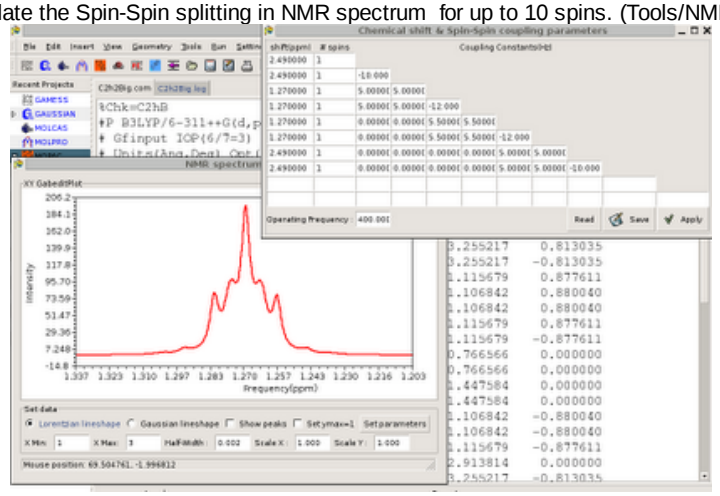


- A XY plotter : Tools/XY plotter. You can read data from a XY file (2 or more columns), JDX or jMRUI files.
  For read data : On the XY plotter window click with the right button and select Data/Add data.
  For change the option for a curve, double click on the curve.
  Using the middle button of the mouse, you can *zoom* in on that interesting feature of *curves.*



- You can read frequencies and intensities from several CCP output file for simulate a UV spectrum (Tools/UV). Similar tools are available for simulate ECD, IR and Raman spectrums

- Gabedit can simulate the Spin-Spin splitting in NMR spectrum for up to 10 spins. (Tools/NMR).



The Gabedit format (.gab)

You can vizualise the results for any computational chemistry packages through a file with Gabedit format

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) values of the density at each point in the grid. Each row contain 6 reals separated by a black space. If N3 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
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-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
.....

Tutorials

A tutorial for Gabedit is available from here

Old manuals

Old manuals in pdf format are available from here