Software News and Updates

Gabedit—A Graphical User Interface for Computational Chemistry Softwares

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Abstract: Gabedit is a freeware graphical user interface, offering preprocessing and postprocessing adapted (to date) to nine computational chemistry software packages. It includes tools for editing, displaying, analyzing, converting, and animating molecular systems. A conformational search tool is implemented using a molecular mechanics or a semiempirical potential. Input files can be generated for the computational chemistry software supported by Gabedit. Some molecular properties of interest are processed directly from the output of the computational chemistry programs; others are calculated by Gabedit before display. Molecular orbitals, electron density, electrostatic potential, nuclear magnetic resonance shielding density, and any other volumetric data properties can be displayed. It can display electronic circular dichroism, UV–visible, infrared, and Raman-computed spectra after a convolution. Gabedit can generate a Povray file for geometry, surfaces, contours, and color-coded planes. Output can be exported to a selection of popular image and vector graphics file formats; the program can also generate a series of pictures for animation. Quantum mechanical electrostatic potentials can be calculated using the partial charges on atoms, or by solving the Poisson equation using the multigrid method. The atoms in molecule charges can also be calculated. Gabedit is platform independent. The code is distributed under free open source X11 style license and is available at http://gabedit.sourceforge.net/.

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Key words: GUI; computational chemistry softwares; animation; charge distribution; electrostatic potential; molecular density; visualization

Introduction

The continuous speedup of computer hardware has made quantum chemistry programs very valuable tools in fields as diverse as drug design, planning, synthesis, and materials science. Predictions from quantum chemistry methods can be considered as complementary to other investigation. However, non-specialists are often discouraged from using these tools due to the use of unfamiliar concepts or complex user interfaces. Experienced computational chemistry software (CCS) users, as well as non-specialists, could benefit from a user-friendly interface that simplifies this step, and then distills important and relevant output from CCS calculations into a convenient format. Some CCS providers simplify the use of their product by developing a specific graphical user interface (GUI). In many instances, optimum study of a given system requires the use of several quantum chemistry softwares, so Gabedit as a single GUI able to assist the user to manage multiple calculations using various quantum chemistry softwares is practical and advantageous.

The quantum chemistry softwares are also used increasingly in education. Having a GUI, Gabedit is easy to use, and is, therefore, well suited as an introduction for students learning to prepare data files (which are often quite complex), to start calculating and learning to analyze the results. Gabedit is a teaching aid, in this context.

Gabedit provides a package to assemble and modify molecular structures in a simple and powerful application. It can generate input files for the most popular CCS including Gamess-US,[1] Gaussian,[2] Molcas,[3] Molpro,[4] MPQC,[5] Open Mopac,[6] Orca,[7] PC Gamess,[8] and QChem,[9] then run the appropriate CCS and finally, analyze the results of these calculations.

The default settings make Gabedit readily accessible to beginners and students, but the default settings can of course be custom-tailored to suit the more experienced user.

The remainder of the article is organized as follows: a description of the general capabilities of Gabedit is followed by

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more in-depth discussions of the geometry builder, the CCS input generator, and CCS output visualization. Finally, a comparison between capabilities of Gabedit and those of other softwares is provided.

Program Overview

Gabedit is a GUI developed 1) to facilitate the production of results from quantum chemistry methods through various CCS and 2) to provide a thorough analysis of these results. It constructs a molecular geometry, from which an input file for any one of the Gabedit-supported CCS packages can be made. It then runs the chosen CCS and provides an analysis of corresponding output.

Gabedit can build the molecule atom by atom, or fragment by fragment. It can also read the geometry from a variety of file formats, as discussed in the section on the geometry builder. Once geometry has been established, the user can create an input data file for any CCS supported by Gabedit. Gabedit contains a text editor and the input CCS data require modification. The user can run the CCS job from the graphical interface of Gabedit, either on the local computer or on a remote host server.

The most powerful features of Gabedit are associated with the analysis it performs on the CCS output files. Appropriate visualization can be a critical aid to the proper interpretation of the results, and also offers a valuable educational tool. Gabedit is tuned to provide real-time visualization with modest hardware requirements, so that the program can run on a standard laptop computer to present results at scientific meetings, or be used in classroom environments for educational demonstrations. Gabedit can produce output in a variety of formats suitable for both hardcopy and Web-based publication as well as screen-based visual formats. These options are described in detail in the section on the output file analysis. Visualization options include simple structures, series of structures, normal modes of vibration, molecular orbitals, total electron densities, density differences, molecular electrostatic potentials (MEPs), and any other volumetric data properties that can be read from a variety of file formats recorded in Table 1. The openGL library furnishes 3D hardware graphics acceleration.

Table 1. LIST of File Formats Supported by Gabedit.

Operation	List of files formats
Read geometry	Output file of any of nine computational chemistry softwares (CCS) supported by Gabedit: Gamess-US, Gaussian, Molcas, Molpro, MPQC, Open Mopac, Orca, PC Gamess and Q-Chem. Input file of Gaussian, Molcas, MPQC, Open Mopac, Orca, PC Gamess and Q-Chem. Gabedit, Molden, XMol XYZ, Hyperchem, Tinker, Mol, Mol2 and Protein Data Bank (PDB), OpenMopac aux, Gamess, and PC Gamess IRC files.
Save geometry	Input file of any of nine CCS supported by Gabedit. Gabedit, XYZ, Hyperchem, Mol2, Tinker, PDB, Mopac Z-matrix or Gaussian Z-matrix.
Read volumetric data	Gaussian cube file (orbitals, density, potential, Laplacian), Molpro cube file (orbitals, density, potential, Laplacian), Gabedit cube file, ADF ASCII tape 41 (orbitals and density), Grid ASCII Molcas file, and Q-Chem grid file.
Export the image in vectorial file format	Geometry, surfaces, contours, color-coded planes, electric dipole, principal axes, XYZ axes, labels, spectrum can be exported in EPS, PDF, SVG files formats.
Save the screen in file	Any window of Gabedit (Draw geometry, OpenGL window, Curves window) can be saved in PNG, JPEG, BMP, PPM files format.

Geometry Builder

Gabedit allows the user to construct a molecule and to examine it in three dimensions (see Fig. 1).

Various possibilities are offered by Gabedit to build the geometry of a molecule. From Gabedit one can build molecules atom by atom, from fragments, or using the tools implemented in Gabedit for building linear molecules, cyclic molecules, molecules with an axis of symmetry, polypeptides, polynucleic acids, polysaccharides, and nanotubes. The structure of a molecule can be imported from an existing file (the file formats supported by Gabedit are listed in Table 1). Gabedit is able to modify the geometry of the molecule in 3D. An XYZ editor included in Gabedit can be used to change the coordinates. Gabedit can convert the XYZ format to a *Z*-matrix format. The *Z*-matrix can then be modified using an editor with which the distance between atoms, angles, dihedral angles, and the connectivity between atoms can all be altered. The values of distances, angles, and dihedral are recalculated automatically after any change of the connectivities.

Gabedit can optimize the structure by a molecular mechanics (MM) calculation implemented in it, using Amber parameters. It can also optimize the structure, interactively, through a semiempirical method using Open Mopac or PC Gamess. The user can perform a molecular dynamics (MD) simulation using a MM potential implemented in Gabedit or a semiempirical potential using Open Mopac or PC Gamess. Conformational searches based on a MD simulation followed by an optimization of structures selected during the MD simulation can be performed with Gabedit. The potential used during the simulation can be a MM or a semiempirical potential.

Most computational chemistry softwares are able to freeze some atoms of the molecule during the geometry optimization procedure. Gabedit allows doing this using a "click to select" operation to specify which atoms are to be frozen.

Gaussian can perform ONIOM[10] calculations, where the molecular system under investigation is divided into two or three layers which are treated at different levels of sophistication. Gabedit accepts a selection of atoms to be considered at a given level, and then the desired level of calculation (low, medium, or high). This facilitates Gaussian ONIOM calculations.

The user-defined geometry can be saved in various file formats, which are indicated in Table 1. This image can be exported in any of the vectorial formats and on a Povray format. Gabedit can also save a screen capture of the geometry to a file. The image can equally be copied to clipboard, to include it in another program such as MS-word, open office, or gimp.

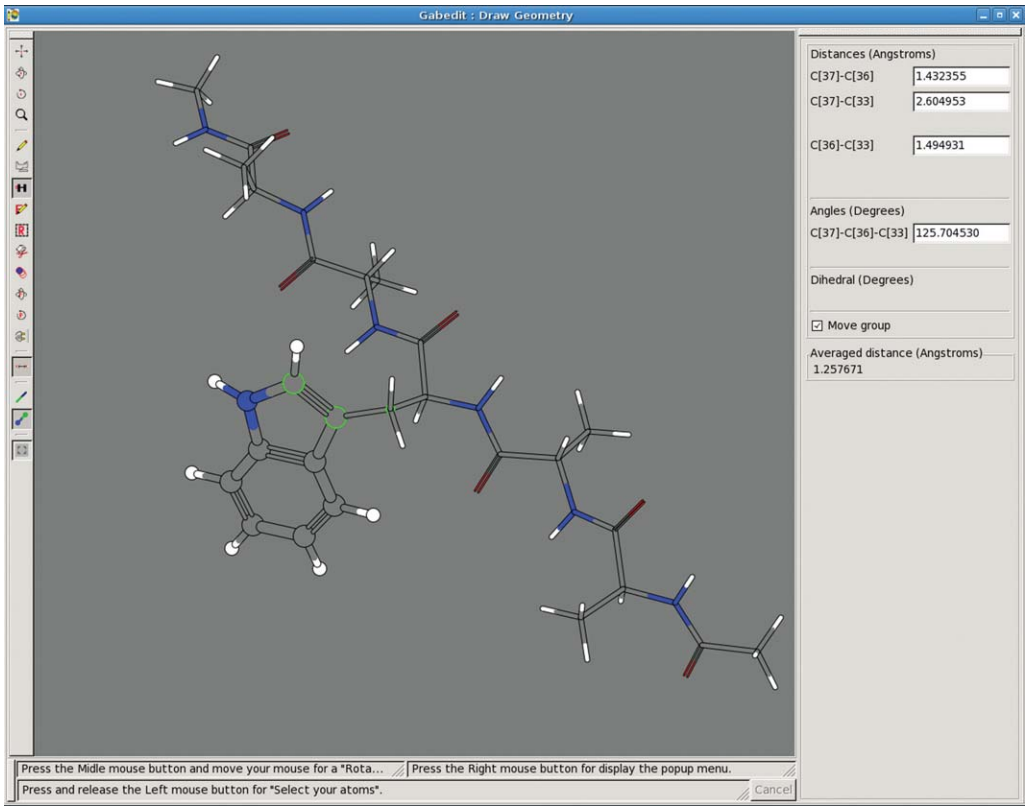

Figure 1. The Gabedit geometry builder window in action.

Once the molecule building step is performed, the user can easily generate an input file for any of the nine CCS supported by Gabedit to date.

Input Generation

Gabedit incorporates an input generator to help construct CCS input files. Figure 2 illustrates the interface of the input builder for Gaussian software. The input groups that are present enable the user to specify the type of wavefunction, basis set, type of run (optimization, internal reaction coordinate, saddle point search, etc.), molecular parameters (charge, multiplicity, symmetry, etc.), and various other options that affect how the CCS will run the calculations.

The constraints on the geometry optimization, defined during the geometry-building step are taken into account when creating the input CCS file. For some CCS, like Gamess, Molcas, and PCGames, one can define the symmetry group in the input file. Gabedit can detect the symmetry and it can remove the atoms that are generated by the CCS according to symmetry group.

Submitting a CCS Job

Having created an appropriate input file, the user can run the CCS job on the local computer or on a remote host server via the graphical interface of Gabedit. Figure 3 illustrates the submission step of a CCS (Orca in this example) job via Gabedit.

If the user accepts the default settings, Gabedit builds a script file (sh under Unix, bat under Windows) and submit a monoprocessor calculation, on the local machine or on a remote machine, following user's choice. However, the user can use his own script file to submit his job with one or more processors. The user script can accept any number of parameters, but the last parameter must be the name of the input file. With the Gabedit source files, it includes scripts (sh) for the most common batch systems, such as load sharing facility, LoadLeveler, portable batch system, and sun grid engine. The user can use these scripts to run his favorite CCS but the user should ensure that these scripts appear in his PATH.

To submit a CCS job under Windows, the user must specify the locations of the directories where the CCS routines are installed, using the settings/preferences options in the Gabedit menu.

Result Analysis

Gabedit processes numerical information produced by CCS. This processing can result in direct visualization, if all the necessary information is available directly. If it is not, additional visualization information may be calculated via Gabedit in an intermediate computational step.

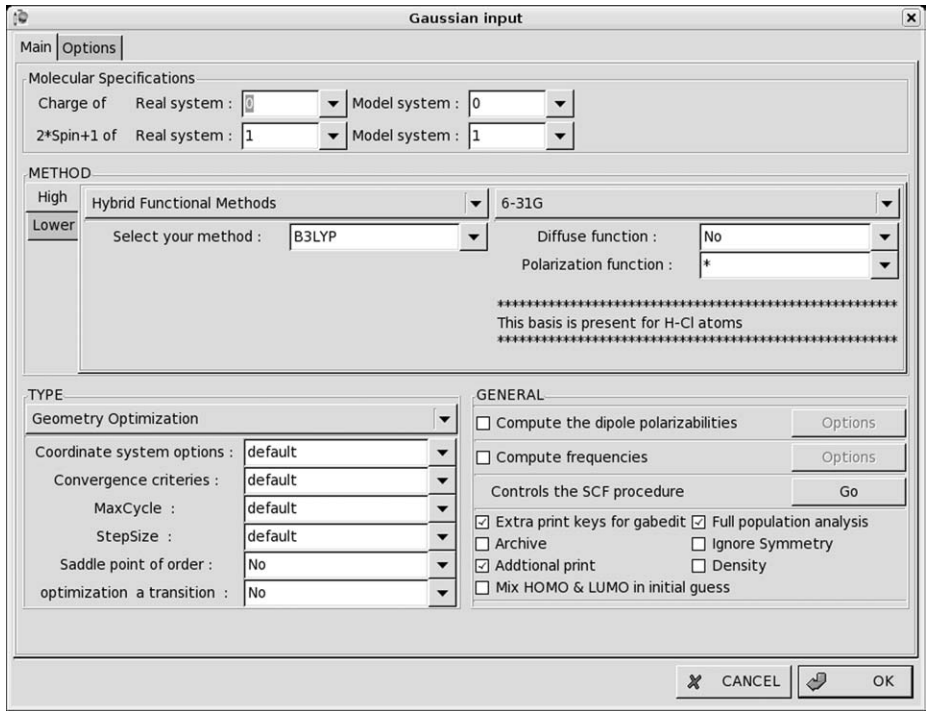

Figure 2. An example to generate input for Gaussian.

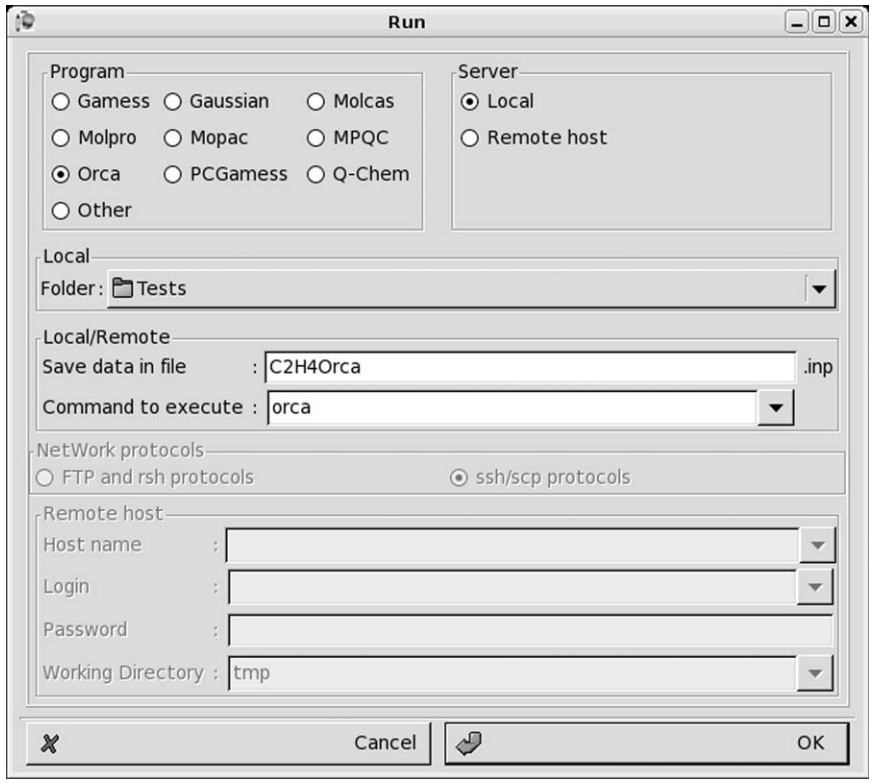

Figure 3. Submission job window.

Figure 4. Vibration vectors for a selected mode of the benzene molecule.

Animation of Computation Results

Gabedit is able to animate computation results. This includes the animation of normal modes as well as any multiframe computation from CCS. Gabedit displays normal modes as a series of geometries. The starting geometry is gradually distorted by scaling the atomic displacement vectors that make up a normal mode. Gabedit allows the animation to be saved in the form of a series of image files (cf. Table 1). These can be converted by external programs (such as "Convert" from ImageMagik) to a .gif or .png animated file. The animation can also be saved in a series of Povray files to obtain a high quality animated file. Gabedit also indicates the vibration vectors (Fig. 4). The minor components can be excluded to avoid cluttering the picture. Gabedit can read the normal modes from the output files of the nine CCS supported by Gabedit, from a Gabedit file, or from a Molden[11] file.

Gabedit can animate reaction paths from internal reaction coordinate calculations, MD trajectories, optimization, and saddle runs.

Analysis of Volumetric Data Properties

Gabedit can visualize any volumetric data properties in a user-defined plane either as a 2D contour map or 2D color-coded plane. It can also visualize these data in a 3D isosurface. Most of the volumetric data file formats can be read by Gabedit. Several volumetric data properties can also be calculated by Gabedit using the molecular orbitals and the atomic basis sets taken from the output files produced by the Gabedit-supported CCS packages. Gabedit can also read the orbitals and the atomic basis sets from a Molden file and (naturally) from a Gabedit format file. Using the orbitals and the atomic basis sets, Gabedit can calculate the following volumetric properties: molecular orbitals, electronic density, electron-localized function, solvent-accessible surface, and spin density. It can also compute the molecular electronic density minus the atomic electronic densities, but in this case, the atomic orbitals must be supplied via a Gabedit file. Gabedit can calculate the MEP from volumetric electronic densities, by solving the Poisson equation numerically, using the multigrid method.[12] Gabedit can also calculate the MEP using the partial atomic charges. Isosurface contours for a chosen volumetric property can be color coded using any other volumetric property (Fig. 5). More options are available to manipulate a volumetric property. For example, Gabedit can square, scale, apply a restriction, compute the gradient, compute the Laplacian (generally used to compute the Laplacian of the electronic density, an important property in the atoms in molecule (AIM) Bader's theory[13]) for the volumetric property (read from a file or calculated by Gabedit). Gabedit can take the difference between one volumetric calculation and another; this feature is generally used to analyze the consequence of electronic excitation.

Using the electronic density, Gabedit can calculate the AIM charges via the method proposed by Tang et al.[14] There are several different approaches to calculate Bader volumes. Early algorithms were implemented for quantum chemistry calculations of small molecules, in which the gradient of the charge density can be calculated from derivatives of an analytic wavefunction, using a linear combination of Gaussian basis sets.[13,15] The method has been criticized as being computationally expensive for large systems. The grid-based algorithm of Tang et al. has been implemented in Gabedit. This method is highly efficient, scales linearly with system size, and is robust to complex bonding topology found in condensed systems and is not limited to wavefunctions where the Gaussian basis sets are used.

Using the gl2ps library, Gabedit is able to export all visualized properties in a 2D vector graphic files formats (Table 1). Gabedit can also export the scene, without the labels, in a Povray file. A screen capture can be saved in a file (Table 1).

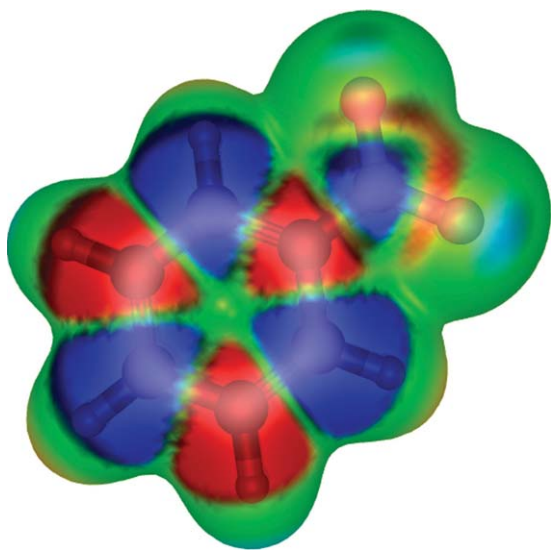

Figure 5. Electronic density isosurface, color-coded with the spin density of $C_6H_5NO_2$ anion, calculated at the UHF/6-31G* level.

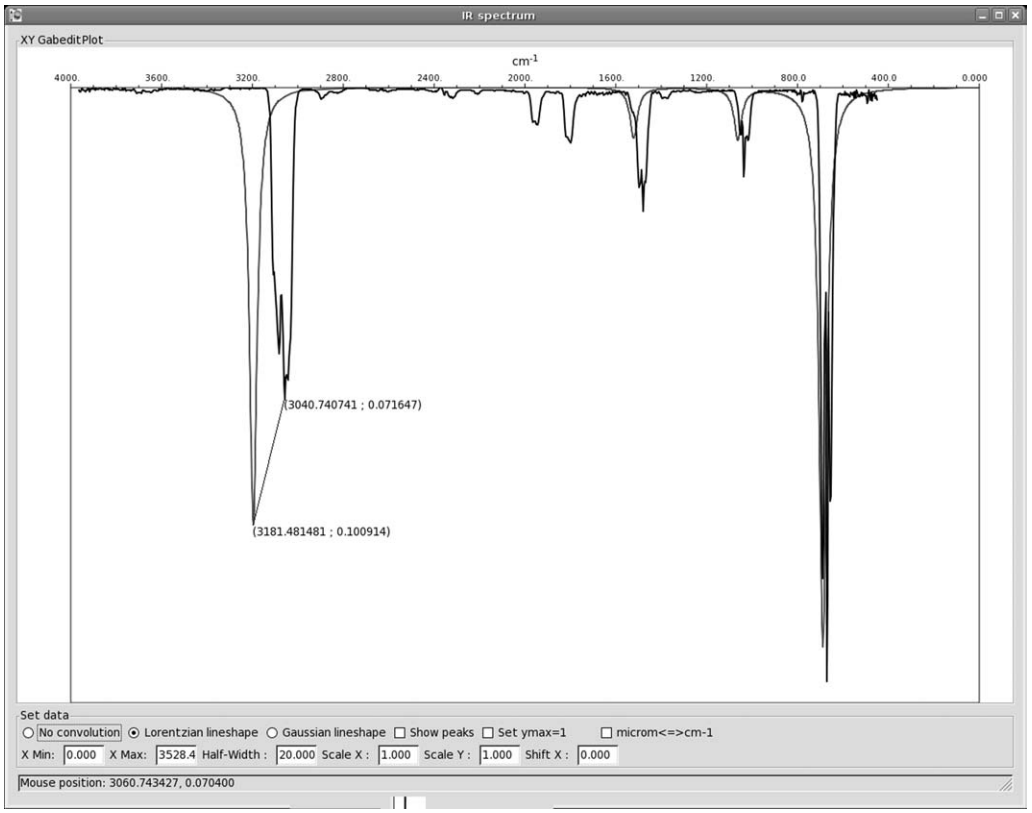

Figure 6. A calculated B3LYP/6-31+G* IR spectrum of benzene molecule, compared to an experimental one (read from a JDX file format).

Other Properties

Repulsion integrals can be calculated analytically or numerically by solving the Poisson equation using the multigrid technique. Permanent electronic dipoles can be calculated using the partial charges or from the volumetric electronic density. The transition matrix between orbitals can be calculated by Gabedit.

The density of states can be calculated (convolution using Lorentzian or Gaussian line shapes) and shown in 2D plotting window, implemented in Gabedit. The half-width at half-maximum, used in the convolution can be changed by the user. The electronic circular dichroism, ultraviolet-visible, infrared, and Raman spectra calculated as peaks by the CCS can be also convoluted by Gabedit, using Lorentzian or Gaussian line shapes. The spectra as peaks and after convolution are shown in the 2D plotting window of Gabedit, where several options are available to edit the curve; scaling, shifting, saving of data on a text file to be used by other graphics softwares, changing of the line style, and more others options. The user can also measure the distance between two points of the 2D window. One can add curve by reading a text multiple columns file, JDX format[16–18] file, and JMRui[19] text file (Fig. 6). Using the chemical shift and indirect spin–spin coupling parameters, Gabedit can simulate nuclear magnetic resonance spectra. The program currently handles a maximum of 10 spin groups to economize computational effort, but the number of spin groups can easily be augmented in the source files. Gabedit is able to export the curves in a 2D vector graphic file formats (Table 1). A screen capture of the 2D window can be saved in a file (Table 1).

Comparisons with Other Softwares

Some distributors of computational chemistry programs have developed a customized graphical interface to facilitate the use of their product. For example, GaussView[20] is a GUI for Gaussian,[2] MacMolPlt[21] is a GUI for Gamess-US,[1] and CCP1[22] is a GUI for Gamess-UK.[23] Each of these interfaces supports only one CCS. Theoretically, to study a given system, the use of several quantum chemistry softwares is often necessary and then a graphical interface that supports the majority of CCS is useful. Several freeware programs have been developed for this aim. The visualization of results is the main objective of some of these programs, such as Molekel,[24] Jmol,[25] and Molden,[26] whereas editing the geometry used in CCS is the main objective of other softwares such as Ghemical[27] and Avogadro.[28] As an application, Gabedit provides a freeware GUI enabling the edition of the geometry, the creation of input files, the submitting of a CCS job, the computation of several properties, and the visualization of the results for nine softwares, among the most popular ones in the field of quantum chemistry. Table 2 gives an overview of the capabilities of Gabedit compared to the Molden

Table 2. Comparison Between Gabedit, Molden (Version 4.8 under Linux) and Avogadro (Version 1.0.0 Under Windows).

Operation	Gabedit	Molden	Avogadro
Tools for building geometry	Z-matrix editor. XYZ editor. Draw molecule atom by atom. Build polypeptides: 24 conformations are available, polynucleic acids, polysaccharides and nanotubes. Build molecule fragment by fragment: about 200 fragments in the database, the user can add his personal fragments. Optimization of geometry by MM or semi-empirical methods. Conformational search based on molecular dynamics simulation, using a MM or semi-empirical potential.	Z-matrix editor.	XYZ editor. Draw molecule atom by atom. Build polypeptides: three conformations are available. Build molecule fragment by fragment: implemented but no fragments are available in the database. Optimization of geometry by MM. Conformational search (based on openbabel) limited to very small molecules.
Creation of input file computational chemistry softwares	Gabedit has a tool to create input file for: Gamess-US, Gaussian, Molcas, Molpro, MPQC, Open Mopac, Orca, PC Gamess and Q-Chem. The consistency between charge and spin multiplicity is controlled by Gabedit. The constraints on the geometry optimization, defined during the building molecule step are taken into account when creating the input CCS file. For some CCS, like Gamess, Molcas and PCGames, one can define the symmetry group in the input file. Gabedit can detect the symmetry and it can remove the atoms that are generated by the CCS using the symmetry group. Gabedit can create an input file for ONIOM Gaussian calculation.	Mopac7: no control of consistency between charge and Molden has a tool to create input file for Gamess-UK, Gaussian, and spin multiplicity. The symmetry is not computed by Molden and the input geometry is for a C_1 group.	Avogadro has a tool to create input file for Gamess-US, and Gaussian. No control of consistency between charge and spin multiplicity. The symmetry is not computed by Avogadro and the input geometry is for a C_1 group.
Run a CCS	Gabedit can run any of the nine CCS supported, locally or on a remote machine. The output file of the CCS can be got from the remote machine by one click.	Molden can run Gamess-UK, Gaussian, Mopac7 locally.	Not implemented.
Quantities calculated before visualization	Molecular electrostatic potential (MEP), orbitals, electronic density, difference density, Laplacian of the density, AIM charges, Fukui functions, ELF, SAS, Coulomb integrals, transition matrix elements. Volumetric data can be scaled, squared or subtracted. The peak IR, UV, Raman, ECD spectra can be convoluted with a Gaussian or a Lorentzian profile. NMR spectra can be calculated from chemical shift and spin–spin coupling constants. Gabedit can calculate the ro-vibrational correction to chemical shifts and to spin–spin couplings. The isotope distribution for a molecule can be calculated by Gabedit.	MEP, orbitals, electronic density, difference density, Laplacian of the density and SAS. The peak IR and Raman spectra can be convoluted with a Gaussian or a Lorentzian profile.	Orbitals, electronic density.
Visualization of results	Gabedit can visualize the geometry, volumetric data as surface, contours or plans color-coded form. It can animate the vibration. The IR, Raman, UV, ECD, NMR spectra (with or without a convolution) can be plotted and compared to other data (a full 2D plotting tool is implemented).	Molden can visualize the geometry, volumetric data as surface or as contours form. It can animate the vibration. The IR and Raman spectra (with a convolution) can be plotted.	Avogadro can visualize the geometry, volumetric data as surface form. It can animate the vibration. The IR, Raman, UV and CD spectra can be plotted as peak form (without a convolution).

and Avogadro programs, which are among the softwares closest to Gabedit.

Conclusion

Gabedit provides an easy-to-user interface for most computational chemistry packages, offering a range of features appealing to the novice as well as the veteran user. Gabedit provides to CCS users a wide range of tools that facilitate the use of these softwares: very powerful and easy to use builder geometry, a tool to create the input files for the CCS, a tool to facilitate the run of the CCS job, and varied tools to analyze at the best the calculation results.

Gabedit produces high-quality graphics output, suitable for publication. It also supports the most popular formats for the publication of results on the Web, such as jpeg, png, and animated png or gif. Gabedit has already established a sizable user base worldwide; 20% of which is used in teaching applications.

Many enhancements are planned for future versions of Gabedit. Among these are plans to support several other CCS not presently supported by Gabedit, including PSI3,[29] DFTB+,[30] and NWChem[31]. Several other tools will evolve to enhance the analytical capacity of the package, for example, a tool to locate and visualize the critical points of the electronic density (AIM Bader theory) and a tool to search the basins of ELF[32] and to integrate the electronic density for each basin.

Availability

Gabedit is available free of charge to all users, on an open source license. To obtain Gabedit please refer to the Web address: http://gabedit.sourceforge.net/. Complete system requirements, feature lists, user manual, several tutorials as well as the program itself can be found at that site.

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