



Introduction to molecular modeling: An inexpensive experience using free software



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Nowadays teaching of computational chemistry is something that can be considered as necessary in undergraduate curricula. However in most institutions this remains as a complementary topic left for seminar or some additional lab classes. Most of the still remaining obstacles frequently claimed by teachers is the cost for licensing software, this one is in most cases very specialized, when sometimes the only aim is to render nice molecule representations, a modern alternative to stereo models in most of their applications, but even in this case this is something worth to be taught and the under graduated students should be skilled in their use.

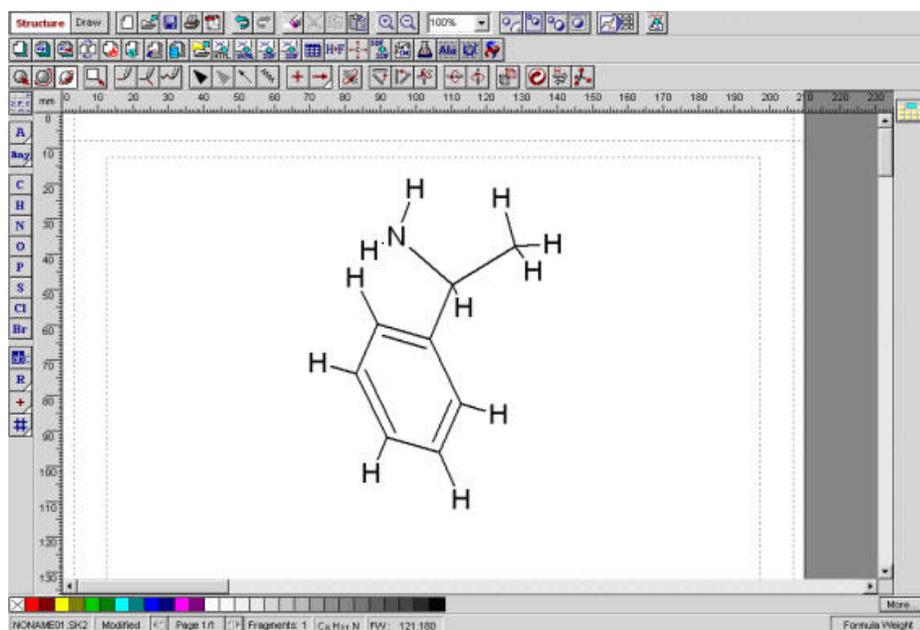
The large number of commercial programs available, could led to think that they are the only tools to teach computational chemistry. However, there are several programs freeware that can be used to build stereo models, and carry out some electronic calculations, with no extra effort by teacher and students.

Rather than presenting here a review on freeware computational chemistry, we shall just present the way we use to teach our undergraduate students the basics of computational chemistry. This is aimed to get a complete understanding on the building of molecules, their 3D existence and properties can be calculated and visualized. The other aim is to set a point to discuss among the teaching community, their experiences in using this kind of software without being skilled programmes, just a point where the state of art could be shared, in a field where the reality is in continuous change.

As a first approach, the simplest use of molecular modeling is to get molecular structures with minimal energy constraint. This process requires a three-dimensional structure to start from, with its corresponding set of coordinates. This feature, included in most commercial programs, can be considered as something that make necessary to buy this software to teach molecular modeling, but as we shall show there are another ways.

Two classic free programs for molecular calculations are the old versions of MOPAC up to [7.21](#), and [GAMESS](#). However they lack of visualization and molecular builder complements (although GAMESS presents [MacMolPlt](#) for macintosh computers. These options to visualize their results are: [MOLEKEL](#), [MOLDEN](#). They allow not only viewing the structures but some electronic properties. However MOPAC 7 and GAMESS are planned to carry out calculations rather than to render nice representations, although last efforts by the developers of [WINGAMESS](#) to interface it with MOLEKEL are really helpful. Another interesting program freeware is [ARGUSLAB](#), the last release is version 4.0.4, but we still use 3.1. This software allows not only doing calculations and visualizing results but it has a built-in builder as well. However, to be used for beginners it is easier to have 2D to 3D conversion automatic. This feature is presented by Chemdraw-Chem3D from CambridgeSoft commercial software very common in organic laboratories. However, there is another choice: use one of two freeware 2D drawing programs that allow to save the molecules as MDL .mol format, ChemSketch from [ACD/Labs](#) and ISISDraw from [MDL](#). These can be directly opened by Arguslab, or converted to MOPAC or GAMESS input files by using [WINBABEL 1.99](#).

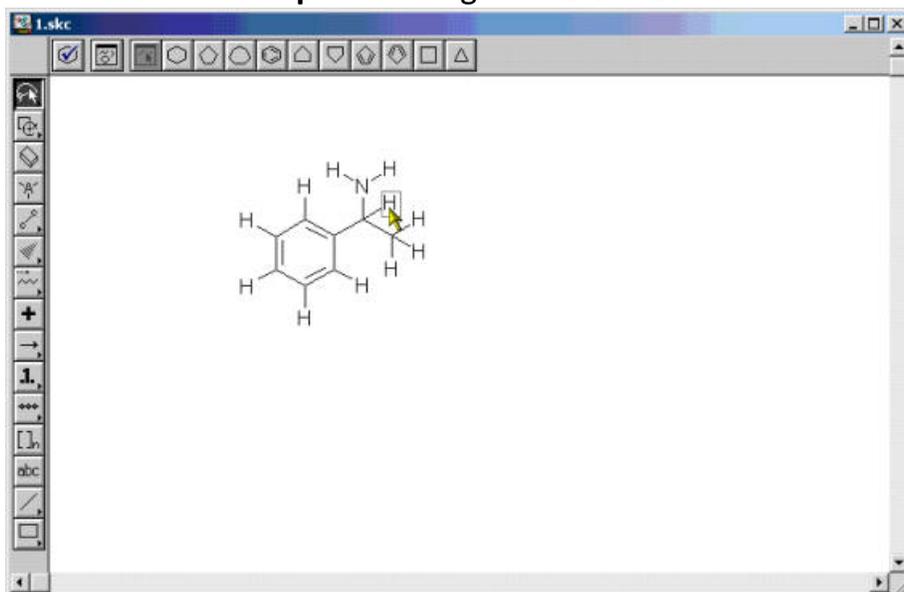
The most direct one is using ChemSketch since it renders a tridimensional structure which can be used directly by argus or translated to MOPAC or GAMESS, and modeling can be carried out with any additional manipulation. Even more, this program allows rotation of the converted three-dimensional structure in the 2D drawing screen. This molecule must be exported as .mol file.



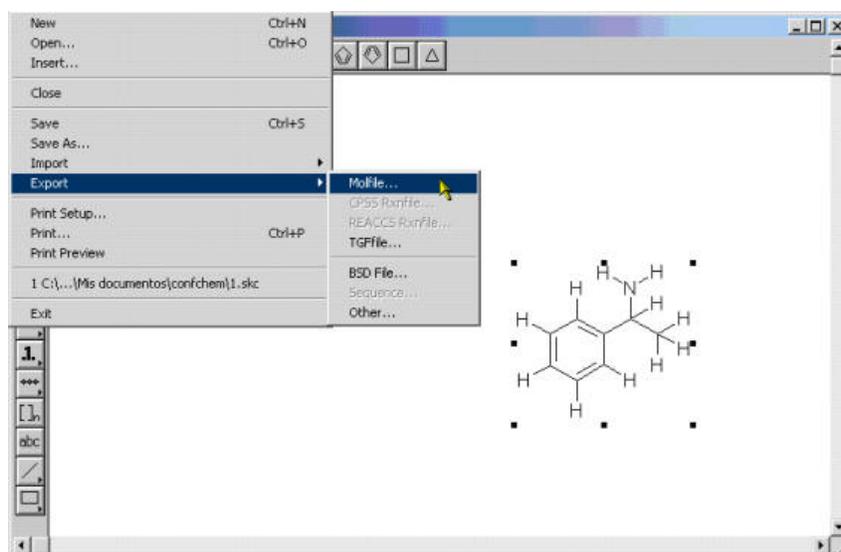
Alfa-phenylethylamine drawn with ChemSketch after converting to 3D.

The use of ISISDRAW, requires more manipulations before the molecule can be used for calculations, since it renders a planar molecules in the .mol file exported. The steps to follow are shown.

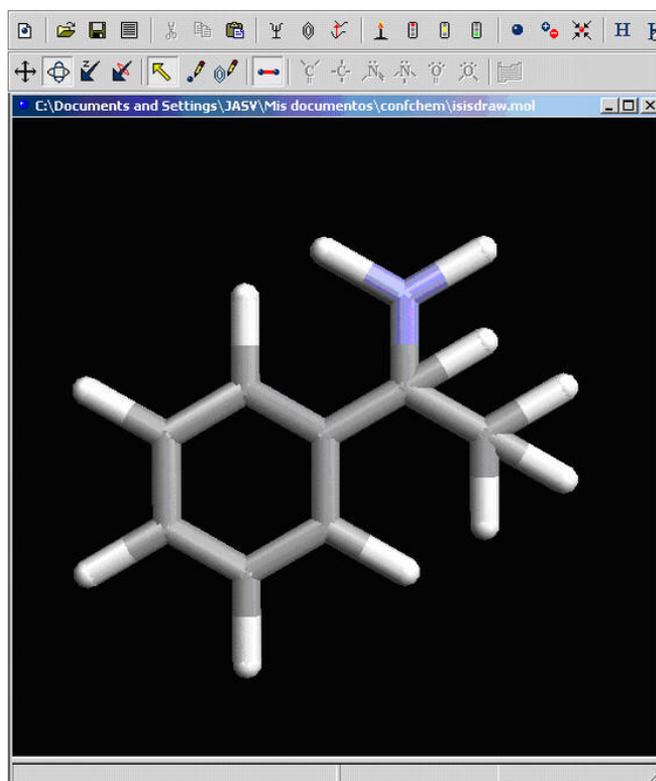
Step 1: drawing 2D molecule



Step 2: Saving the molecule as 3D coordinates

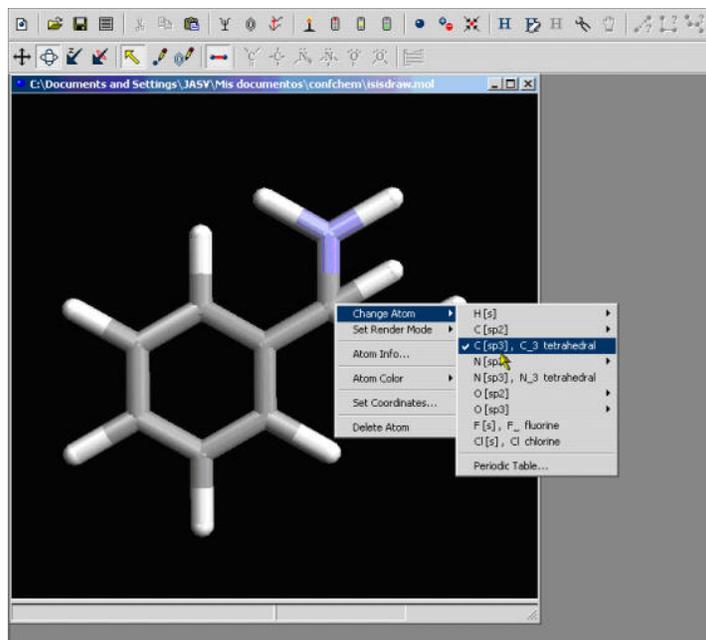


Step 3: Opening the coordinates file with arguslab.



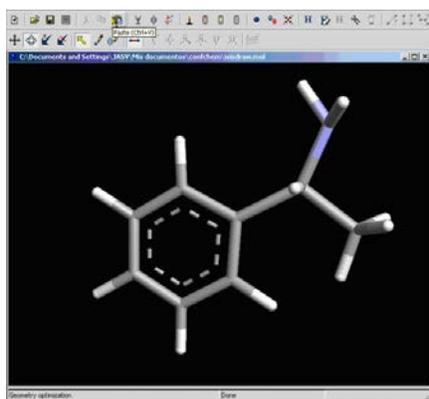
The program will open a planar molecule. Here the student has to check the atom parameters of the molecule opened (hybridization, bond order). This is easily done by selecting atoms or bonds, and changing their parameters with a menu which appears when right button of the mouse is pressed.

Step 4: checking the structure



Step 5: Getting a clean structure

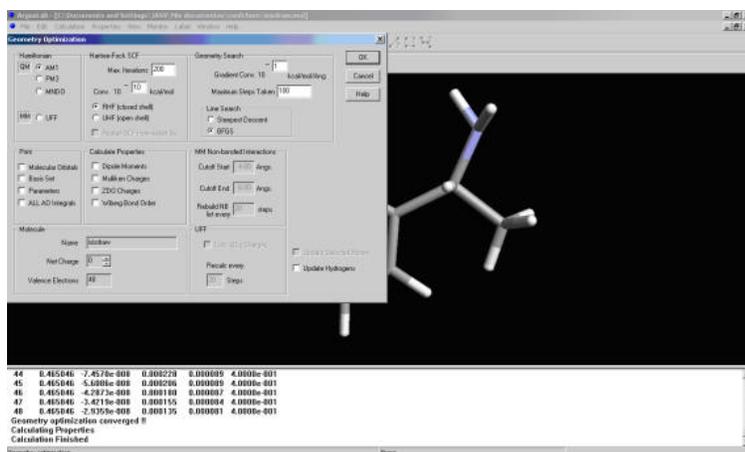
Once everything is checked the molecule can be optimized to render geometry according to the structure.



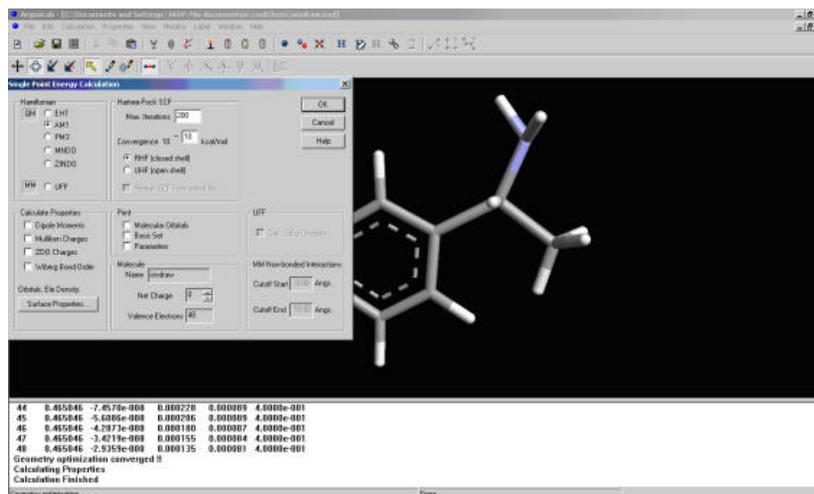
CALCULATIONS

Arguslab allows carrying out semi empirical calculations:

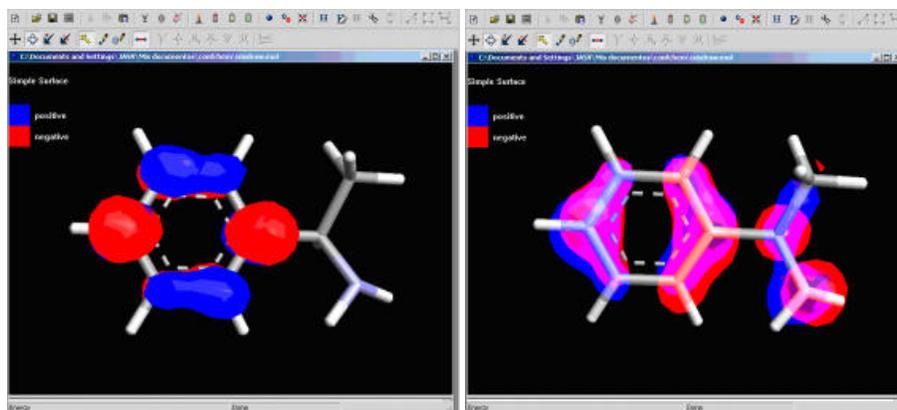
geometry optimization



Single point energy calculations

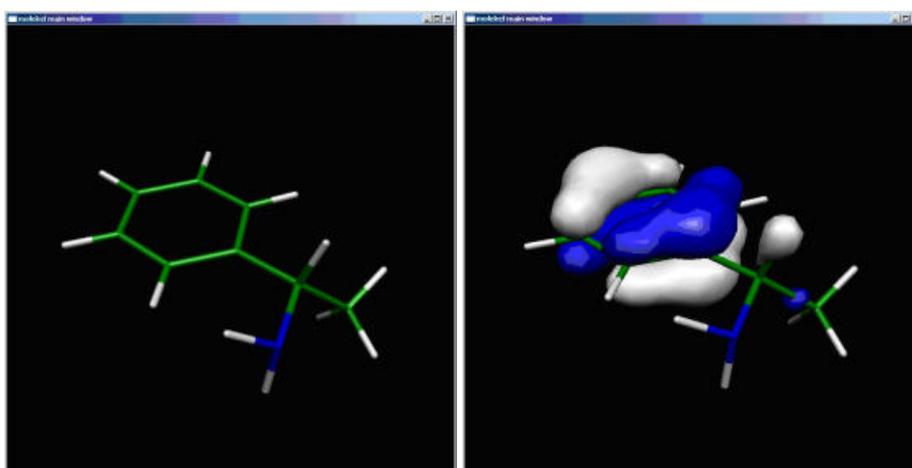


These are implemented by a surface visualization with good display quality.

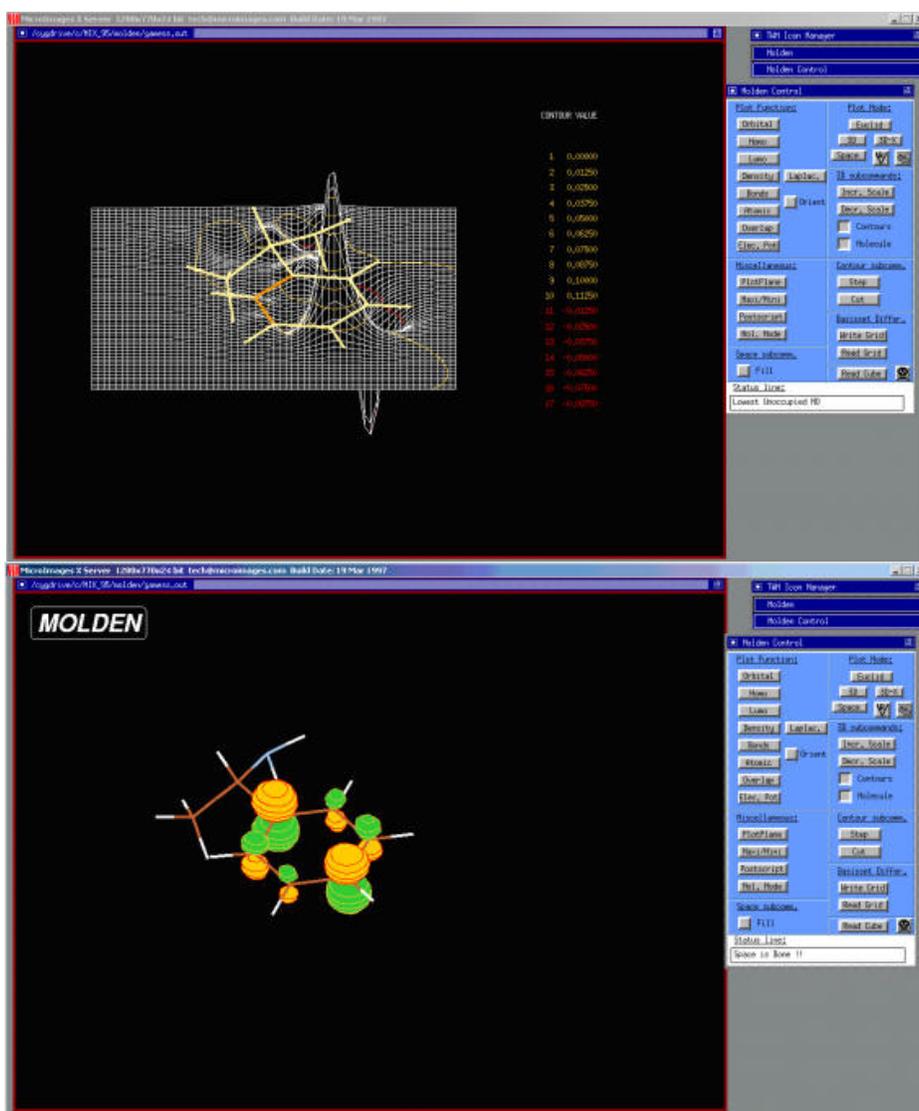


Calculations to predict UV-vis spectra, however this feature is out from our teaching purposes.

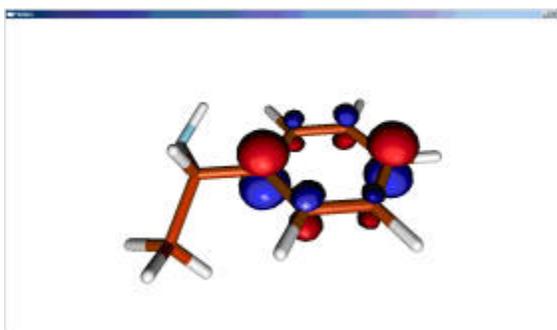
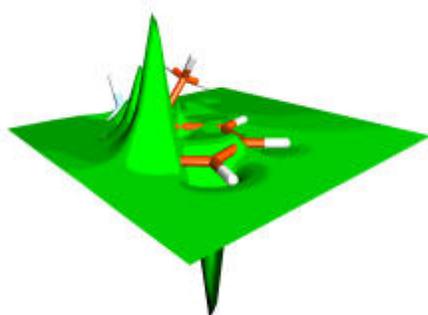
A good choice for semi empirical and ab initio calculations is GAMESS, the method we used consists in preparing an optimized structure with ARGUSLAB, convert its coordinates to GAMESS and then using WINGAMESS to carry out the calculations. The results can be visualized with MOLEKEL or with MOLDEN. Both are good visualizing programs, however MOLEKEL does not read MOPAC output files, while MOLDEN requires X-WINDOWS system which can run with freeware [CGWIN/X](#).



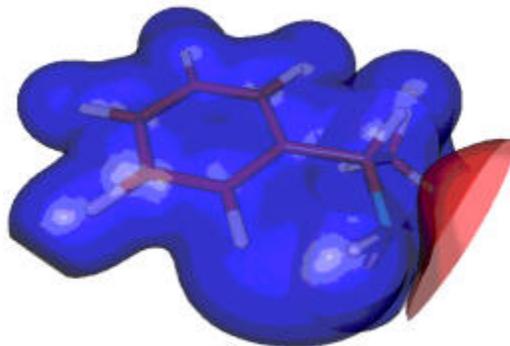
Screenshots of molecule and homo orbital with molekel.



Screenshots from molDen, showing two different rendering styles for orbitals



OpenGL rendering from molden.



OpenGL rendering for electrostatic potential.

In summary our communication tries to make a contribution to the general teaching of computational chemistry, looking for being the starting point towards the globalization of computational chemistry in all educational institutions regardless their economic inputs.

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