Your Web Browser as a Computational Chemistry Frontend

Handling quantum chemical programs can be tricky and their input files are quite often rather cryptical. Not only do you need an overview of all the keywords. Usually you also have to struggle with their general syntax: "Do I need a comma or an equals sign here?" The outcome is always the same: The program crashes, you waste computer time, and so on.

WebMO tries to put an end to this. On the basis of Netscape & Co., a graphical frontend has been developed with the intention to make life easier. You can draw your molecule with the mouse, select the quantum chemical program package (Mopac, Gaussian, and Gamess are currently supported), and finally generate the input file through pulldown menus. Just a few mouse clicks and that's it. You can submit and control the calculation through your browser. After the calculation is completed, the most important results will be extracted from the output file and will be readily presented to the user. Molecular vibrations can be visualized and with the commercial WebMO Pro, you can even plot molecular orbitals, electrostatic potentials and so on quite nicely on the screen (Figure 1). What more could you possibly need?

But who belongs to the clientele of this product? When I had the idea to compute pyridine *N*-oxide—by no means the most exotic molecule—I experienced a number of surprises. For example, the molecule editor offers the appealing feature to generate useful geometry parameters for the drawn molecule. However, the procedure behind this is by no means plain to see. And why the nitrogen atom should be sp^3 is beyond my understanding! Consequently, I came up with the idea to import a preoptimized structure from an xyz file. The program gave me the message "Molecule successfully imported", yet I could not find it anywhere. How can I obtain a useful input geometry? No way! I am obliged to leave the geometry as I drew it and proceed. In order to get an optimized structure, I want to perform a B3LYP/cc-pVDZ optimization using Gamess. This means that I have to select "Gamess" and "Geometry Optimization". But how can I select the density functional? Most likely under "Theory / other"—but that did not work either and I thought I had chosen a standard method. Now I focus on the basis set. I cannot find cc-pVDZ in the pulldown menus. Instead, I read entries such as "Basic: 3-21G" and "Routine: 6-31G(d)". Well, 6-31G(d) is still used quite often but an entry "Basic: 6-31G(d)" would be more appropriate. But how can I select the cc-pVDZ basis? Not even by using "Basis set / other" since cc-pVDZ is not in the Gamess basis set library. Does WebMO not even have its own basis set library? For that reason, I had to enter 6-31G(d,p) but with spherical d functions, and in order to do so I looked up the keyword in the Gamess manual. Wait a minute, isn't that exactly what a frontend should help to avoid? And how can I finally perform my DFT calculation? Fortunately, there is a "Preview Input File" button, which gives me the possibility to edit the input file manually. This way, I manage to prepare my input for a B3LYP run. But what do I need WebMO for if I have to write the input file by hand in the end? This way, I could go on complaining about many other faults and insufficiencies regarding the information extracted from the output, job submission, and so on. And providing RHF/3-21G as default parameters is by no means up to date. Of course, the visualization of the molecular orbitals and the electrostatic potentials is appealing but many public domain programs do the same for free. Besides, WebMO does not work properly under Netscape 6.2.

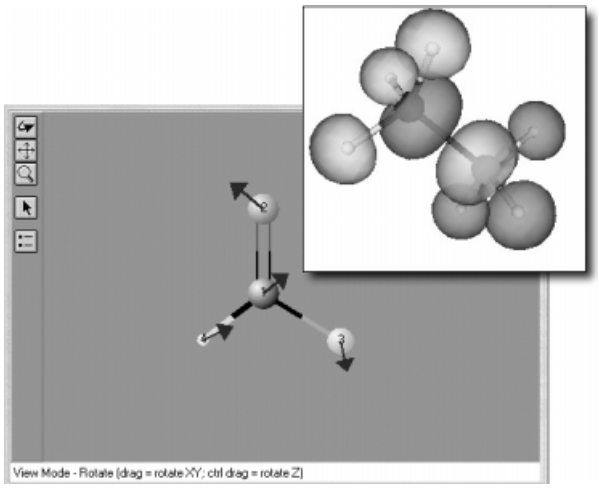

Figure 1. Some visualization features in WebMO: vibrations and molecular orbitals.

Suggest a web site or submit a review:
angewandte@wiley-vch.de

Although not new, the idea behind WebMO definitely is a good one and a powerful frontend program would be very helpful for many users. However, if the frontend is not even able to handle standard calculations—for which in principle I wouldn't even need a frontend—the question remains: What is an academic user such as myself supposed to pay US$ 995 for? Personally, I would rather buy a new computer from that money and carry on writing inputs by hand.

Guntram Rauhut
Universität Stuttgart (Germany)

For further information visit:
http://www.webmo.net
or contact
polik@webmo.net

  1433-7851/02/4112-2205 $ 20.00+.50/0