HyperChem Release 3 for Windows

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Hyperchem is a blend of tools which will find useful application over the whole range of users from high school student to university professor. The program allows one to select from well-integrated features which smoothly combine two- and three-dimensional graphics with molecular mechanics and semiempirical quantum calculations. The "point and click" environment is friendly and easy to use, and the applications should span the whole range of subjects from fundamental physical chemistry to macroscopic biochemistry.

REQUIREMENTS

System requirement may be intimidating for the small-school user. The package requires Windows 3.1, a 386 or higher processor (with a 387 or DX), at least 4 MB of RAM (6 MB is recommended) at a cost of $595 dollars (assuming an academic discount). The copy protection leaves no doubt that Autodesk takes the protection of their software seriously, as the installation requires a "hardware lock" be placed between your printer port and the printer cable. HyperChem boots successfully only with the lock in place, while the lock itself remains transparent to any other application.

INSTALLATION AND HELP

Often when using new software for the first time, I will deliberately not read manuals and tutorials to see what I can do aided only by the clarity of the menus and icons. HyperChem does not disappoint, and one finds most of the CAD-type features for drawing molecules very easy to grasp. The installation was friendly and flawless, menu driven at each step, and easy to follow without the manual. Note: the comments made in this review are based on installation and use on a CompuAdd 486DX2 with 8M of RAM, a 200-MB hard drive, and SVGA graphics. After installation one may use an available tutorial to learn the package. It is concise and to the point, introducing you to each feature of the program with examples available for inspection. On-line help is exhaustive and easily toggled from the menu bar for "search" or by topic.

CONSTRUCTING AND DISPLAYING MOLECULES

Drawing molecules for presentation is the most basic feature HyperChem offers. Perhaps because of Autodesk's previous work on "Autocad", here lies one of the strongest features of the package; simple mouse-driven operation allows one to place atoms with the left button or erase them with the right button. Changing the atom being placed involves only a double click on the placement icon, which brings a periodic table into view as a removable window. One clicks on the atom desired, and that atom remains the default until you select another. Creating bonds is also easy, done by "clicking and dragging" between the atoms being linked. Left click and right click

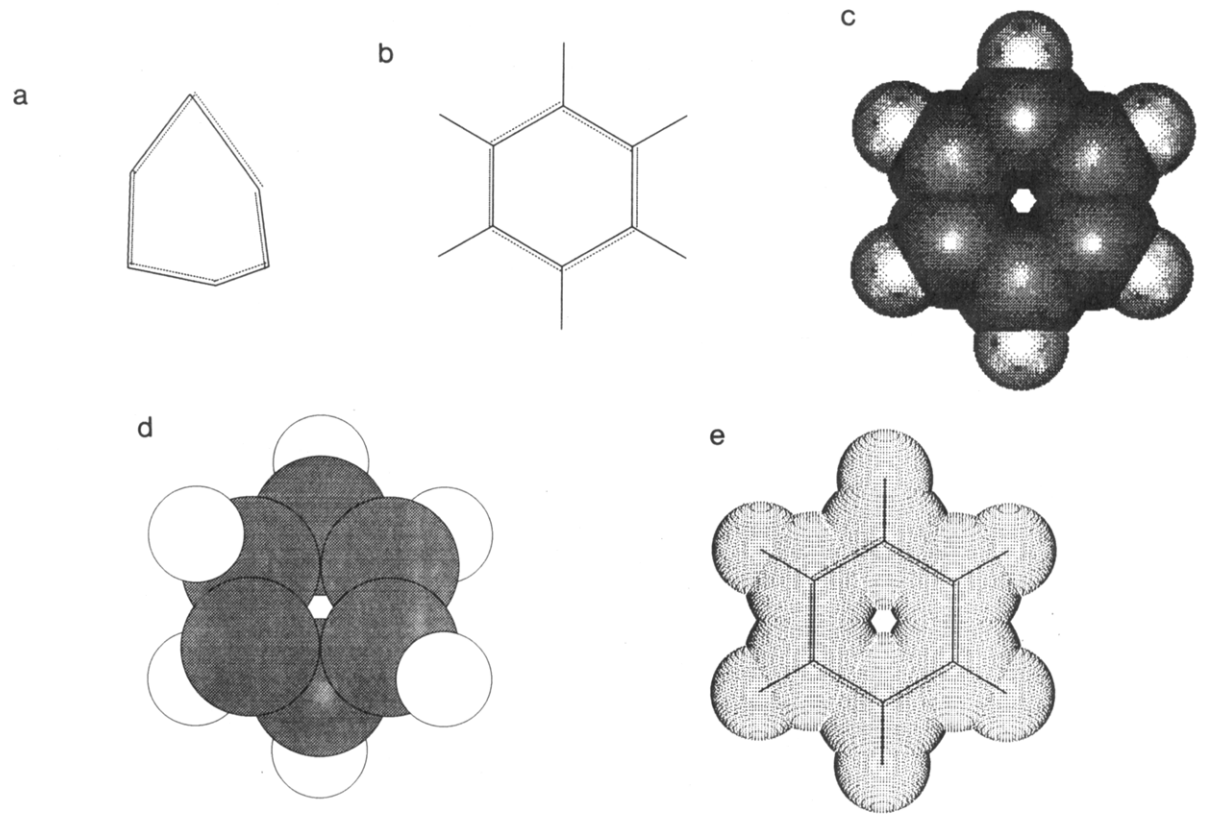

Figure 1.

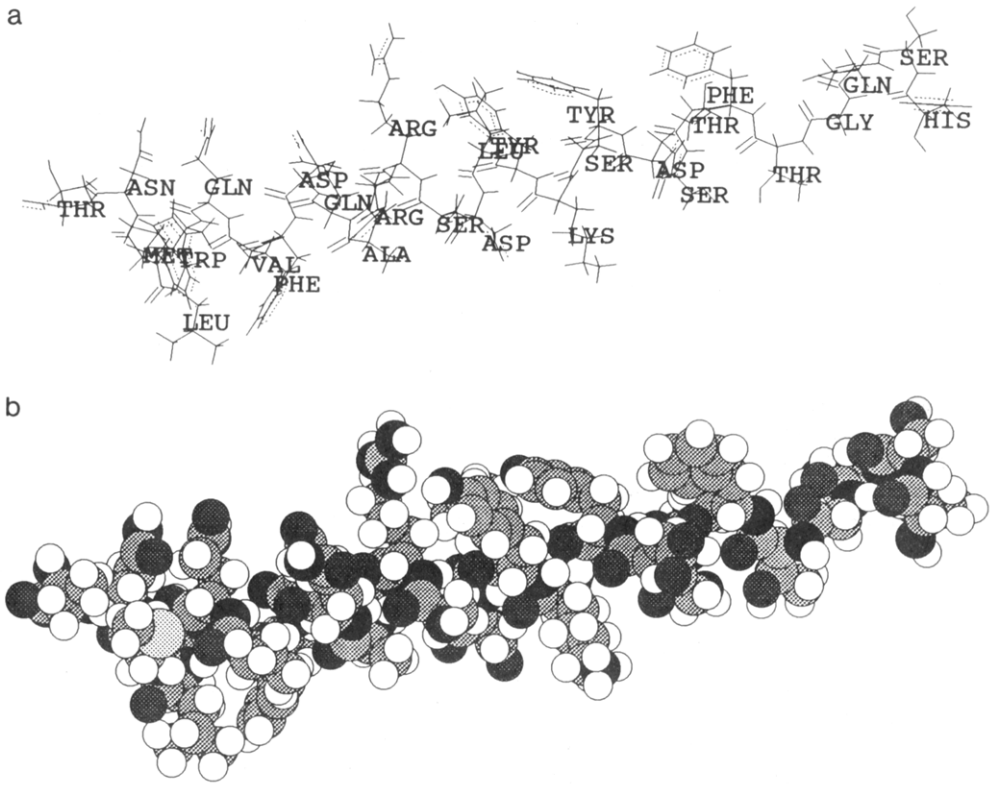

Figure 2.

toggle bond order up and down, while left or right double click on the mouse adds or removes aromaticity. Using benzene, the process is illustrated in Figure 1. First the basic skeleton is built (and it need not be neat, see Figure 1a). The conversion of a 2-D rough sketch to a 3-D structure requires only one menu selection, the "model builder". This tool arranges the atoms in the most reasonable presentation and fills in carbon valence with H if requested (see Figure 1b). The presentation can take several alternate forms, as shown in Figure 1c (spheres), 1d (discs), and 1e (dots and sticks). The 3-D representation of the molecule may be easily zoomed (in and out), rotated (along x, y, or z axes), or "sliced" (along any plane) using icons from the "tool bar" which are clearly labeled. Once a molecule is displayed in this fashion it is also a "one click" operation to obtain bond angles, bond distances, or absolute coordinates of any atom in the structure.

MACROMOLECULES

Manipulation of macromolecules is also straightforward. To begin, toggle the "Database" menu option to "Amino Acids" and the "Select" menu option from "atoms" to "residues". In analogous fashion to the point and click construction of simpler molecules, one may link amino acids by simply clicking on the three letter abbreviation. Once the sequence of amino acids is complete, one may select α helix, β sheet, or other (specify specific Φ, Ψ, and Θ) as well as the D or L isomer. A huge collection of biochemical structures (*.hin PDB files) are available free of charge via electronic mail or anonymous FTP from the Brookhaven Protein Databank (BPD; pdb.pdb.bnl.gov). Figure 2 shows a file that I downloaded from BPD for illustration (plant seed protein crambin) in two different display formats. Figure 2a uses the stick display with each residue labeled (labels are prohibitive for most large proteins; they obstruct the structure), while Figure 2b shows the same molecule in 3-D disc format.

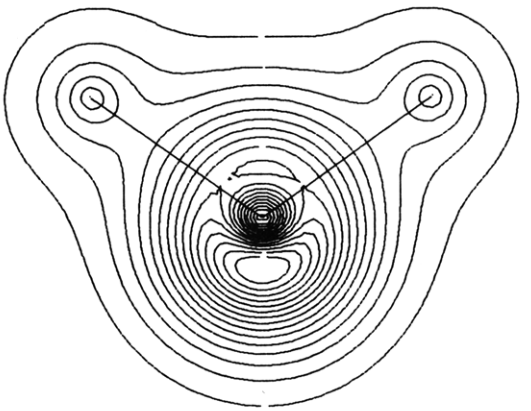

Figure 3.

CALCULATIONS AND RELATED DISPLAYS

The calculation features offer molecular mechanics using MM+, AMBER, BIO+ (CHARMM), or OPLS. Quantum calculations are available using HUCKEL, CNDO, INDO, MNDO, AM1, PM3, and ZINDO. Calculations can take several minutes (especially for MM+), but the results I calculated for known systems were accurate (bond angle in water, C–C distances in various organics among others). Menu options allow the user to plot molecular orbitals, electrostatic potentials, total charge density (see Figure 3 for an example using water), and total spin density. Geometry optimization can be done several ways beginning with rough estimates using "steepest decent" to more accurate results using "Newton–Raphson" or "Polak–Ribiere". With recording on one may specify boundary conditions and allow multiple species to interact to create a "movie" of molecular mechanics (such as $H^+ + H\text{–}H \rightarrow H\text{–}H + H^+$ which is available in the built in script for demonstration). Similarly one may take a system (such as a protein) and anneal to a lower energy minimum by selecting the time, temperature, and heating or cooling. Again, this operation may be saved for later use as an edited

demonstration by selecting "playback dynamics" that meet your specific needs. HyperChem may also be operated out of Excel or Visual Basic, although these options were not examined.

SUMMARY

Although not as powerful as the package of tools one might have at their disposal using a fully equipped Silicon Graphics environment, HyperChem provides a set of tools that span the pedagogical needs of the high school or college student at a fraction of the cost (one can imagine creating the whole system from nothing with about $2000). Most students should be able to master the techniques and topics relevant to their study fairly quickly and easily. The display formats available combined with an overhead projection system makes HyperChem an excellent lecture and demonstration aid. Overall, HyperChem is an excellent piece of software.