COMPUTER SOFTWARE REVIEWS

HyperChem Release 4.5 for Windows

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INTRODUCTION

The 10th anniversary of Hypercube, Inc., is marked by the release of HyperChem 4.5 for Windows, which gives the user the possibility to perform ab initio quantum mechanical calculations on a PC. HyperChem is a molecular editor and a computational chemistry package, which offers a wide range of molecular and quantum mechanics calculations. The powerful molecular editor allows the user to generate in a short time the three-dimensional structure of any organic compound, from small molecules to bioorganic polymers and macromolecules. Once generated, the user can apply to a molecule a wide range of single-point, geometry optimization, and molecular dynamics computations using molecular mechanics, semiempirical, and ab initio quantum methods. The computation results can be inspected with the aid of the powerful graphical tools of the package. This software meets the needs of a wide range of users, from undergraduate and graduate students to academic or corporate researchers, with applications from physical chemistry to organic chemistry and biochemistry.

The program is Windows-based and provides user friendly pull-down menus and an extensive help for easy use of the many features of HyperChem.

SYSTEM REQUIREMENTS

The recommended minimum system configuration for running HyperChem 4.5 is as follows: an IBM PC 386 or compatible with math coprocessor, 6 MB of RAM, a hard disk with at least 20 MB free, and a mouse. To benefit from the graphical capabilities of HyperChem, a color display with at least 256 simultaneous colors is recommended.

The computer must have installed DOS 3.1 or later and Microsoft Windows 3.1. Complete installation of HyperChem requires 12 MB of hard disk space for the program files and 3 MB for the sample files. In order to take full advantage of the new ab initio features of HyperChem, the user must take into account that a large hard disk space is needed to store two-electron integrals for ab initio calculations. The size of the required hard drive space increases dramatically with the increase in the number of basis functions, and it is recommended to have more than 100 MB or even a second hard disk to store the ab initio two-electron integrals.

The evaluation of HyperChem 4.5 reported in this review is based on installation and use of an IBM PC 486 DX2 compatible computer at 66 MHz with 16 MB of RAM, 200 MB of free space on hard disk, and color SVGA display.

INSTALLATION, HELP AND DOCUMENTATION

The installation of the software was straightforward and follows the usual procedure of Windows-based programs. All phases of installation are menu driven and easy to follow without reading the documentation.

The software can be launched by double-clicking the HyperChem icon. Before using HyperChem, one has to install to the parallel port of the computer the hardware lock which comes with the manuals and disks. While using the software, an exhaustive on-line help is available from the menu bar for information on a specific topic.

The printed documentation is extensive and very helpful, consisting of more than 1200 pages in four manuals. The four manuals are well-written and illustrated with many reproductions of screens and dialog boxes. The Getting Started manual contains information on installing the software, system requirements, product support, and 15 lessons with step-by-step instructions for building molecules, performing molecular and quantum mechanics calculations, and creating links with other Windows applications using the dynamic data exchange feature of Windows. The manual ends with an index which covers the topics discussed in the lessons.

The Reference manual discusses in detail HyperChem features and procedures, with many examples, figures, and pictures of the dialog windows. Also, the manual presents in-depth information on the structure of files used by HyperChem, allowing the user to add new parameters in the force field and quantum chemical files.

The textbook Computational Chemistry provides an overview and introduction with examples to the calculations that can be run with HyperChem and a technical reference section with detailed information on the specific implementation of the mechanic and quantum molecular methods.

The Release 4.5 New Features manual describes the new features of the release 4.5, including three new tutorials, the description of the ab initio computations with HyperChem, a description of the other new features, an extensive reference describing the details of the changes to the interface, the script commands, the description ab initio files, and a chapter on basic ab initio theory.

OPERATING THE SOFTWARE

Because HyperChem release 2 for Silicon Graphics and release 3 for Windows were recently reviewed in this journal,[1,2] we will present a short description of the features of the package, with a larger space for the new features of the release 4.5.

Constructing and Displaying Molecules. One of the strongest features of the HyperChem package is the easy construction of the three-dimensional structure of molecules. Using simple mouse-driven operations, a 2-D sketch of a molecule is drawn in the workspace. The conversion of a 2-D sketch to the corresponding 3-D molecular structure requires the use of the Model Builder, which can add also the required hydrogen atoms. The Model Builder is a very powerful tool for 3-D structure generation, which prepares the molecule for the computations. We have used this tool to prepare the 3-D structure for almost one thousand acyclic, cyclic and cage organic molecules, and the Model Builder offered excellent results. The 3-D molecular structure can be presented using a variety of models: sticks, spheres, discs, or dots and sticks. All molecular representations can be easily rotated, zoomed, or sliced. The construction of proteins and nucleic acids is straightforward, by the use of corresponding library of residues from the Databases menu. HyperChem uses rules for connecting these residues to make biomacromolecules.

Molecular Mechanics and Semiempirical Quantum Chemical Calculations. HyperChem offers four force fields for molecular mechanics simulations: MM+ (a modified MM2 force field), AMBER, BIO+ (an implementation of CHARMm force field), and OPLS. Semiempirical quantum chemical calculations are available by the use of the extended Hückel method, CNDO, INDO, MINDO3, MNDO, AM1, PM3, ZINDO/1, and ZINDO/S. Menu options allow the user to plot molecular orbitals, electrostatic potentials, total charge density, and total spin density.

HyperChem can perform three types of calculations: single-point, geometry optimization, and molecular dynamics simulations. All three types of calculations may be performed by using any molecular or quantum mechanical method, with the exception of the extended Hückel method which can be used only for single point computations.

HyperChem has a very useful capability of doing mixed semiempirical/molecular mechanics calculations. In a large molecule, a fragment can be treated at the semiempirical level, while the rest of the structure is fixed and treated as a classical static field. This is extremely useful for treating, for example, the active site of an enzyme, when it would be prohibitive to include the whole system. With HyperChem one can calculate the IR vibrational and UV−visible spectra, thus obtaining useful information for structure elucidation and identification.

The size of the molecules which can be computed depends on the method used and the amount of available RAM memory. We have tested the computational methods on a large number of molecules, with good results. With the computer used for the evaluation, we were able to optimize the geometry of large molecules like the C_{60} fullerene.

Ab Initio Calculations. The addition of ab initio calculations makes HyperChem one of the most complete molecular modeling software for IBM PC computers. In order to carry out an ab initio calculation with HyperChem, one has to follow three steps. First, prepare the starting geometry of the molecule, either with the Model Builder or refined with a molecular mechanics or semiempirical method. Second, assign a basis set to the molecule. Third, apply a calculation method to the molecule. One can perform an ab initio computation for a whole molecular system or only for a part of it. The boundary of the mixed model occurs between molecules.

HyperChem supports a large number of commonly used ab initio basis sets: STO-*x*G and STO-*x*G*, where *x* takes values between 1 and 6; *y*-21G, *y*-21G*, and *y*-21G**, where *y* takes the values 3, 4, and 6; *z*-31G, *z*-31G*, and *z*-31G**, where *z* takes values between 4 and 6; 6-311G, 6-311G*, and 6-311G**; D95, D95*, and D95**.

A very flexible option of HyperChem enables one to use multiple basis sets in a single molecular system. By selecting an atom or a group of atoms the user can apply to the selected part of the molecule a particular basis set. Also, the extra basis function option can be used to add an S, P, D, SP, or SPD shell to the selected atom(s). Different extra basis functions can be applied to different atoms, but any atom can receive only one extra shell. The user can modify a basis set file and create a new basis set, using the extensive information on the structure of basis set files given in the documentation.

Both RHF and UHF ab initio calculations can be performed, according to the molecular system. Single-point, geometry optimization, molecular dynamics, configuration interaction (CI), and vibration calculations are all available with ab initio SCF simulation. With single-point calculations, one can use also the Möller−Plesset second order perturbation method. After the computation of a wave function via the ab initio method, the user can plot contour diagrams of the molecular electrostatic potential, the total electronic density, the spin density, the molecular orbitals, or the electron densities of individual orbitals. After a CI computation, the user can display the calculated UV−visible spectrum, and after a vibrational calculation one can display the theoretical infrared spectrum. Detailed results of the computation can be obtained by using a log file, which can be inspected after the computation is finished.

Three new tutorials are presented in the Release 4.5 New Features manual, in order to emphasize the new ab initio options, thus enabling the user to perform a variety of simple molecular modeling calculations. The first tutorial present the computation of the geometry and energetics of H_3O^+ and the determination of the protonation energy. The second explores the vibrations of ammonia and the differences between the pyramidal and planar form of ammonia. The third tutorial investigates the electronic excitation spectra of ethylene. All calculations in the tutorials can be made in a few minutes, and we found the examples suitable to include in teaching demonstrations.

All the ab initio features are easy to use and robust, and for small molecules the convergence is obtained in a few minutes. However, for larger molecules, requiring extensive use of the hard disk for the storing of two-electron integrals, the computations were run overnight and on weekends.

OTHER NEW FEATURES OF HYPERCHEM RELEASE 4.5

The new release of HyperChem allows the user to investigate the isotope effects in vibrational calculations, both for the semiempirical and ab initio methods. This option is not available for the molecular mechanics calculations.

HyperChem can import files produced by ChemDraw (developed by CambridgeSoft Corporation). The user can copy images of the molecular orbital energy level diagram

and of the vibrational or UV−visible spectra, either to the Clipboard or to a file. The images can be stored either as a bitmapped or Windows metafile format.

SCRIPT FILES AND DYNAMIC DATA EXCHANGE

With HyperChem the user can automate repetitive tasks by the use of a script, which is a file sending instructions and messages to HyperChem. The script file is created with a text editor and consists of a sequence of commands which control the execution of HyperChem. The commands available in a script duplicate the HyperChem functions plus a few commands that are not available with the dialog boxes or menu items.

Using the Windows Dynamic Data Exchange (DDE) HyperChem can be integrated with other programs that also run in the Windows environment. Through DDE, a program can interact with HyperChem by sending commands, requesting information, and collecting the computation results. Some new messages, variables, and commands were defined in release 4.5, mainly for the new ab initio features. Also, new one- and two-dimensional array variables allow the user to control the atomic coordinates and selection and to obtain information on the molecular orbitals and IR and UV−visible spectra.

The script commands are easy to use and flexible, and we found them particularly useful for computations on large sets of molecules, when we have performed the computations overnight, with the results collected in a log file.

SOFTWARE DISTRIBUTION

HyperChem Release 4.5 for Windows is produced and distributed by Hypercube, Inc., 419 Phillip St., Waterloo, Ontario, Canada N2L 3X2; Tel. (519)-725-4040; Fax: (519)-725-5193; information hot-line: (800)-960-1871; E-mail information requests: info@hyper.com; E-mail support questions: support@hyper.com. The software is reasonable priced, when compared with the quality and the number of computational methods: 1295 U.S.$ for academic users, and 2595 U.S.$ for commercial users. To obtain HyperChem, contact one of the Hypercube dealers; the address of the nearest dealer can be obtained from Hypercube.

Hypercube maintains a World Wide Web site at http://www.hyper.com. The new products and releases are announced there as well as auxiliary materials which can be downloaded via ftp. Also, there is a HyperChem Internet E-mail Users' Group, where users can share their experiences and ideas in order to improve their use of HyperChem. To become a subscriber of the users' group, send the message "subscribe hyperchem" to hyperchem-request@hyper.com.

CONCLUSIONS

The computational methods implemented in HyperChem 4.5 are very robust, and we have encountered no convergence or other numerical problems after extensive use of the features of the software. My experience with HyperChem both in teaching and research is very favorable, and I would rate the program excellent on this category of software. HyperChem is easy to learn and use, and with a little practice one can investigate the compounds of interest with a large number of molecular and quantum mechanics methods. The molecular visualization and simulation tools implemented in HyperChem makes an excellent software for education and research, with a low price/performace ratio, and requiring the now widely available PC computers.

REFERENCES AND NOTES

(1) Bearden, D. W. HyperChem Release 2 for the Silicon Graphics Workstation, *J. Chem. Inf. Comput. Sci*. **1993**, *33*, 525−528.
(2) Pazun, J. L. HyperChem Release 3 for Windows. *J. Chem. Inf. Comput. Sci*. **1993**, *33*, 931−933.

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