THE TEKTRONIX CAChe SYSTEM

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During July of 1991 two Tektronix CAChe workstations became operational at St. Olaf College. A new era of accessibility to computational methods in chemistry at the undergraduate level began. In this article I will describe (1) the features of the CAChe system, (2) our specific configuration and its cost, (3) why we chose it for use in our program, (4) how we have used it thus far, and (5) some advantages and disadvantages of the system.

Hardware

The Macintosh II series of microcomputers serves as the basic platform for the CAChe system. We chose specifically the Macintosh IIfx with 8 MBytes of memory because of its overall power and flexibility, although less powerful Mac II series computers could be used. Tektronix will sell the computer as part of the overall package, but we found it to be significantly cheaper to purchase the IIfx through St. Olaf's computer center. The real computational horsepower for the CAChe system comes from the RP88 coprocessor board that Tektronix furnishes with the system. A board fitted with 8 or 32 MBytes of RAM may be selected, the memory amount of which dictates the number of atoms that can be accommodated by the MOPAC application (*vide infra*).

A 16-inch monitor equipped with polarizing screen enables the operator to visualize molecules in three dimensions if he or she wears special glasses. Molecules displayed on the screen literally seem to jump out at the viewer and provide a spectacular effect for the novice and experienced user alike. For small molecules it is usually not necessary to use the stereo display mode; we have found that students tend to tire of it after an initial fascination with the 3-D effect. The stereo option is not a slick gimmick, however. I find that using it is essential when dealing with even moderately complicated structures because it allows me to easily select specific atoms for further manipulation on the screen. Structures and structure fragments are maneuvered readily through use of a trackball that allows scaling to most any size as well as rotation and translation along the x, y, or z

axes. Selections from menus and some aspects of structure editing are controlled by the mouse and keyboard.

Completing the list of hardware options available with the CAChe system is a printer. We selected a Tektronix Phaser SX color wax printer that produces high quality prints and transparencies. Other wax and inkjet printers are suitable and available from Tektronix. Both workstations access the same printer through an inexpensive local area network.

Software

Tektronix supplies software with the workstations that consists of a series of seamlessly interconnected applications. These applications operate similarly to any Macintosh program, and persons already acquainted with the Mac will find their use straightforward.

The "Molecular Editor" serves as the keystone of the CAChe software. Using the mouse; shift, option, and "apple" keys, and various "tools", the user can rapidly enter molecular structures on the screen. The "atom" tool opens up the periodic table so that any atom may be incorporated into the structure with appropriate charge, hybridization, and user-defined color. Structure input is enhanced by the fact that Tektronix has already provided over 200 structures or fragments of structures (simple rings, amino acids, DNA bases, transition metal ligands, and many more) in the "fragment" tool. By judicious selection of fragments and subsequent connection of them together, molecule input can be fast and efficient. The "select" tool allows one to select all or part of a structure for additional editing. Bond angles, bond lengths, and dihedral angles may be selected and locked if desired. Final clean-up of the drawing is accomplished through use of the "beautify" tool whereby invocation of pre-defined rules for valence and geometry provide a structure that seems to have minimum energy.

Connected to the "Molecular Editor" are the "Molecular Mechanics" and "Molecular Dynamics" applications. Tektronix uses a set of energy minimization parameters based on Allinger's MM2, but extends these parameters to include all atoms in the periodic table. Steepest Decent, Newton-Raphson, and Conjugate Gradient methods are available for the calculation. A rather impressive option in the "Molecular Mechanics" applications is the production of an energy map. Serving as a particularly simple example of this option would be rotation about the C_2-C_3 bond of butane. The number of rotations and the angle for each rotation may be specified with the condition that

each conformer generated is energy minimized. The resulting calculations are translated into a "map" file that can be visualized as a split screen. One side of the screen shows the energy map (in this case the map is simply a two-dimensional energy vs. angle of rotation diagram such as appears in many organic chemistry texts) and the other side displays the conformer corresponding to the angle of rotation. Using the mouse one may select any point on the energy map, and the conformer corresponding to that point is instantly displayed. The user may also choose to animate the display of energy vs. corresponding conformer. If more than one bond is chosen for rotation or more than one bond angle selected for systematic deformation, a 3-dimensional map is produced. This is a superb tool for teaching students about conformation analysis.

The CAChe system can perform molecular orbital calculations at either the extended Hückel or SCF semi-empirical level. No *ab initio* capability is available at this time. The "Extended Hückel" application incorporates parameters for all atoms in the periodic table and is a product of the CAChe group. The calculation produces an ASCII output file containing eigenvalues and eigenvectors that can be printed out or edited in a word processor (we have Microsoft Word). More impressive, however, is to send the output to the "Tabulator" application where the results of the MO calculation are converted into image files. These files can be shown as pictures of the various MOs in the "Visualizer". The "Visualizer" application resembles the "Molecular Editor" in that MO pictures can be modified and manipulated on the screen and viewed in 3-D if desired.

Semi-empirical SCF calculations are provided under MOPAC (developed by J. J. P. Stewart) and through ZINDO (Professor M. C. Zerner's Intermediate Neglect of Differential Overlap program). MOPAC calculations are limited by the number of atoms (40 hydrogen and 27 non-hydrogen atoms with an 8 MByte RP88 coprocessor and 70 hydrogen and 66 non-hydrogen atoms using the 32 MByte version of the accelerator board). Moreover, only 10 (MINDO/3) to 25 (PM3) different atoms have been parameterized depending on the basis set chosen. The calculations under MOPAC may be done using MINDO/3, MNDO, AM1, or PM3 basis sets. As with extended Hückel, MOPAC produces an output file that may be edited or sent to the "Tabulator" and then to the "Visualizer". ZINDO is parameterized for most of the transition metals since it can use *d* orbitals, whereas MOPAC uses only *s* and *p* orbitals. Tektronix states that ZINDO is faster at geometry optimization, but the geometries obtained are probably not as reliable as those from most of the methods in the MOPAC package. While MOPAC can be used to generate vibrational spectra, ZINDO

may be parameterized to produce spectra in the UV/visible range. Again, results from ZINDO may be ported as an ASCII file or tabulated and visualized in a manner similar to the other CAChe MO applications.

An appealing application within the "Molecular Editor" is that which allows the operator to build crystal structures. The user can either supply the appropriate parameters to build the crystal or can import the data using the "CAChe File Translator" application (*vide infra*). Once the structure is generated, it can be manipulated just as any structure in the "Molecular Editor". Moreover, within the lattice generated the asymmetric cell, unit cell and lattice boundary may be displayed. The crystal building option is an excellent teaching tool for demonstrating important aspects of crystallography.

The "CAChe File Translator" allows importation of structure data files using the Brookhaven, Cambridge, Shelx, Tribble, or Chem3D formats. CAChe molecule files can be outputted as Brookhaven, Chem3D, or Tribble files.

Configuration and Cost of the CAChe System at St. Olaf College:

2-Macintosh IIfx computers each with 160 MB hard disk, 8 MBytes of RAM, and extended keyboard	$11,484
2-Tektronix CAChe Stereo Reactivity Modeling Systems including monitor with polarizing screen, trackball, RP88 25 MHz Co-processor, CAChe video card, and CAChe software .	$44,924
1-Tektronix Phaser II SX Color Printer	$ 4,564
1 Year of on-site printer service	$ 422
Total	$61,394

1. We chose not to subscribe to software updates for the first year ($995/year/workstation) with the assurance from Tektronix that we could elect to receive updates after one year.

2. The prices quoted above are university discounted prices.

3. The printer thus far has been trouble free.

Why We Chose the CAChe System

In November of 1989 a representative from Tektronix demonstrated a CAChe workstation to chemistry faculty and students at St. Olaf College. We were all quite impressed with the system, especially the straightforward user interface. It was instructive for me to see the look in the eyes of the students as they watched the demonstration and played with the system. There was no question in my mind that the CAChe system would appeal to them were we to purchase it for the chemistry department. Although we looked at other hardware and software packages, we kept returning to the CAChe system because it combined ease of use, reasonable computing power, several interconnected calculational methods, and an impressive screen and print output. Most students at St. Olaf who are computer-aware use Macintosh computers. The overriding concern for us in the chemistry department was thus user friendliness. We wanted to purchase a system that was easy to learn to use by faculty and students especially and that would be appealing to use on a continuing basis. This expectation has been met so far.

The Use of the CAChe System

Once the CAChe workstations arrived, it was quite straightforward to get them up and running. Last fall I spent time teaching faculty and interested students how to use the system. During the spring term at St. Olaf the CAChe system has been an integral part of an advanced organic chemistry course that I teach. For every homework assignment and examination, use of the CAChe workstations is required. Thus far we have performed MO calculations at the extended Hückel and AM1 level. We have used the "Molecular Mechanics" application to minimize isomeric structures, calculate coupling constants, and compare calculated values with experiment. Toward the end of the course we will cover concerted reactions using aspects of the CAChe system to compare transition state geometries and to make predictions of product distributions. Next year another course, which covers quantum mechanics and spectroscopy, will employ the workstations to learn about extended Hückel and SCF MO calculations. In future years we also hope to incorporate use of the CAChe system into our advanced inorganic and biochemistry courses. I am presently developing an exercise for our sophomore organic lab course where we can expose students to the workstations in at least one experiment. Several faculty members have used the system to produce drawings and transparencies for classroom use.

The CAChe system is a fine research tool in addition to becoming an integral part of our curriculum. I will briefly describe a project where I have been involved and indicate how the CAChe system has and will continue to assist the research. In collaboration with a member of the biology department at St. Olaf, I have been interested in phytoalexins, which are substances produced by plants to help ward off microbial infections. Phytoalexins may be toxic because of an interaction with cell membranes that causes ion leakage across the membrane. We are developing a structure-activity relationship for various phytoalexins and structural modifications thereof. The CAChe system is helping us to determine what features on the molecule are significant in causing a biological response. MO calculations provide electron density maps and energy minimizations allow us to compare geometries of similar molecules. We plan to purchase a new software package from Tektronix that predicts octanol/water partition coefficient values of molecules. We can use this information to correlate reactivity with lipophilicity and thus try to assess if propensity for interaction with a cell membrane is truly an important component of phytoalexin activity.

Advantages and Disadvantages of the CAChe System

From our standpoint the only major disadvantage of the CAChe system might be its relatively high cost as compared to some of the hardware-software combinations now on the market and described in other articles in this series. When we first seriously considered integrating chemical calculations into our curriculum, these low-cost options were not really available. The last year has seen rather dramatic lowering in prices of computing facilities suitable for 4-year institutions. We were fortunate, however, to receive the requisite funding through an NSF-ILI grant that was matched by funds from the Camille and Henry Dreyfus Foundation as well as other money sources. Another deficiency is the lack of an *ab initio* package; perhaps that will be available in the future.

Calculation speed may be an important consideration to prospective users. The following benchmark calculation speed figures, using the 25 MHz RP88 coprocessor at single precision, were supplied to me by the CAChe Group at Tektronix:

Benchmark	*Speed*
whetstone	24.4 Mwhet
mflops (peak)	7.17 Mflops
mflops (average)	3.31 Mflops
Dhrystones 1.1	53,097

Readers will have to judge for themselves how these figures compare with other systems. To us speed is not an overriding concern, while it might well be in a graduate school or industrial setting.

The major advantage of the CAChe workstations is their user-friendliness. I know of no other system that is as easy to use. Moreover, the applications are linked seamlessly and execute efficiently. Systems management is straightforward because the heart of the system is actually a Macintosh computer using version 6.x or 7 of the operating system. The output to the screen or printer is beautiful and easy to obtain.

Here at St. Olaf College we feel that the advantages of the CAChe system far outweigh any deficiencies, and we are most happy to have such computing facilities on board. If you are interested in an effective, user-friendly, Mac-environment computing system for performing molecular calculations, the CAChe system is well worth considering.