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Comparative review of molecular modelling software for personal computers

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INTRODUCTION

The cost of software and the mainframe hardware necessary for the conformational analysis and molecular modelling of both small (less than 500 atoms) and large molecules can still be prohibitive for some institutions and research groups. However, with recent developments in personal computers (PCs) and the associated hardware technology, molecular modelling has become a tool affordable by most researchers in the chemistry and biochemistry fields, both in the laboratory and at home. Thus it is hoped that this comparative assessment of molecular modelling software available for PCs will provide valuable guidance for investment in such software.

In terms of hardware, the usual PC systems used by the scientific community are Apple, Apple-Macintosh, IBM, and IBM-compatible PCs. The largest variety of modelling software is available for the IBM systems; thus the following packages have been acquired for the purpose of this review: CRYS-X [1], ALCHEMY [2], CAMSEQ/M** and CAMSEQ/PC [3], MGP [4], MOLGRAF [5] (available in both Apple II and IBM versions), and PROMODELER I [6]. A Molecular Graphics' program for Apple computers (also available for IBM PCs) has been reviewed previously [7]. All these software packages fit the $200–1,000 price bracket; PROMODELER I [6] may also be obtained as a hardware/software package. Only CRYS-X (incidentally on the cheaper side of this range) is supplied with source code (Microsoft Fortran), a great advantage to anybody with specialist applications development in mind.

All these packages will run on IBMs (PC, AT, XT or compatibles), with at least 512–640 K-bytes of processor memory, under the MS-DOS operating system. Two 360-Kbyte and/or 1.2 Mbyte $5^1/_4''$ floppy-disc drives are essential. Most of the packages require an Enhanced Graphics Adaptor (EGA) card with 256 Kbytes of extra memory and a compatible monitor; however, some

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**Only CAMSEQ/M was made available for the evaluation.

also support the Color Graphics Adaptor (CGA: CRYS-X, CAMSEQ/M) or Hercules (CAMSEQ/M), while PROMODELER I supports the Professional Graphics Adaptor (PGA) card. Hard-copy requirements differ, with each package supporting different printers. Screen dumps, however, (shift PrtSc key) are possible with each package. In systems with a CGA card, screen dumps are accessible by loading an appropriate driver from MS-DOS (either GRAPHICS or CRTDUMP) prior to running the modelling package. For systems with an EGA or PGA graphics card additional software is required, due to the higher screen resolution. A screen-dumping program, PIZAZZ [8], was also successfully tested with the hardware set-up in our laboratory on which all the software packages discussed (except PROMODELER I, which requires a PGA card) have been installed. This set-up consists of a NEC APC-IV with 40 Mbytes hard disc (APC-H4010), 1.2 Mbytes (APC-H4200) and 360 Kbyte floppy discs (APC-H4210), 640 Kbytes of CPU (central processor unit, Intel 80286-8) memory, EGA graphics card with extra 256 Kbytes of memory (NEC-AGB H-4410), resolution 640 × 350 pixels, eight colours, math coprocessor (APC-H4520, Intel 80287), multi-sync colour monitor (APC-H431x). An Epson FX-100 printer is also attached.

CRITERIA USED IN THE ASSESSMENT

In assessing the modelling software, one should pay attention to the following points.

(1) Ease of use (user-friendliness, documentation, on-line help facilities, whether menu-driven or using input commands consisting of strings from the keyboard).
(2) Structural input, including structure building from atoms or fragment library, structure modification, and possibly minimization, interfaces (file conversion) available to other modelling and/or minimization programs.
(3) Structure display (stick, ball-and-stick, space-filling models, stereo display, global rotations, translations, definition of colour scheme, ease of individual structure manipulation with multiple structures displayed).
(4) Structure comparison (method of rigid or flexible structure fitting).
(5) Conformational analysis (rigid torsion rotations, display of energy profiles or contours).
(6) Electrostatic potentials and/or surfaces.

For any serious modelling, some sort of potential-energy estimation is essential, especially when comparing different conformations of a particular molecule. The fastest calculable energy potential involves the summation, over the whole molecule, of pairwise atomic interactions, as described by the van der Waals term and possibly supplemented by an electrostatic (Coulomb) term. Atomic charges are needed for the latter, and none of these packages is able to evaluate such charges. The Lennard-Jones or mixed Lennard-Jones/Buckingham potential [9] is commonly used for describing the potential-energy term, and is calculated using various force-fields.

Giglio parameterization [10] is used in CRYS-X, White's force-field [11] is adopted in ALCHEMY, and Weintraub's field in CAMSEQ programs [12]. The potential energy in ALCHEMY also contains bond-stretch, angle-bend, out-of-plane bend, and torsion terms. CAMSEQ/M does not include any energy calculation; however, the parameterization potential used in CAMSEQ/PC should include a Lennard-Jones potential, a torsional, an electrostatic, and hydrogen-bonding term. MGP, MOLGRAF and PROMODELER I do not provide any energy calculation.

RESULTS OF THE EVALUATION

We shall now address each of the above points (except the last, which is not available in any of the packages tested) in detail.

1. Ease of use

An on-line help facility is available in all the packages except MOLGRAF. The documentation provided is also quite good, with adequate tutorials or demonstration sequences outlined to enable familiarization with the program. In terms of user-friendliness, both ALCHEMY and PROMODELER I lead, with effectively laid-out menus (comprehensible without reference to the documentation), and mouse pick-up. The only disadvantage in ALCHEMY is that the boxes used for menu pick-up are too small, so that skilful mouse operating is required for quick operation of the program.

These programs are closely followed by CAMSEQ/M, which has similar options and pull-down menus, most of the menu commands also being accessible from the keyboard. An advantage of CAMSEQ/M is the ability to adjust the picking tolerance of the mouse. MGP is also mouse- and menu-driven, with complementary input possible from the keyboard. However, the keyboard commands seem unnecessarily complex, rigid and often not comprehensible without reference to the documentation.

In comparison CRYS-X, which is operated exclusively from the keyboard, has a simple, easily learnt set of commands which covers the essential operations.

MOLGRAF is again menu-driven, but only via the keyboard. Thus getting to a command that appears three or four levels below the main menu may be rather tedious.

No problems were experienced with installing any of these packages, as the instructions and documentation supplied were well written and easily understood.

2. Structural input

ALCHEMY also has the best structure-building facilities, being supplied with an extensive (and easily expandable) fragment library. There are functions for ring fusion, bond-making/breaking, torsion-angle alteration, and the control of stereochemistry. It is the only program which identifies chiral centres and determines whether they are *S* or *R*. These centres, or the whole molecule, can then be easily inverted. Atom types are automatically assigned when building fragments or elements are picked up, and hydrogens can be automatically added or deleted. ALCHEMY is the only one of these packages containing a 3D structure-minimizer, which is very convenient, especially when building complex ring-systems. The potential-energy function used in this ring minimizer includes bond-stretch, angle-bend, out-of-plane bend, torsion, and van der Waals terms. The various parameter files are accessible through the PC's editor, so that new parameters may be added when required. Up to ten molecules (10–50 atoms each) can be comfortably displayed on the screen, although the software limit is probably higher. The ASCII files containing atomic coordinates, connectivity and other parameters may be read or written via ALCHEMY or the PC editor; however, file input is unfortunately a fixed format. ALCHEMY can also create and read SYBYL [13] format files.

CAMSEQ/M provides an interface to the MM2 [14], SYBYL and MDL [15] programs. Structures can also be read in from the ASCII file in the form of fractional coordinates, and CAMSEQ/M then performs the conversion to Cartesian coordinates. For building structures it again uses 3D templates (fragments) or continuous 2D drawing. Structure building and conversion to a fully three-dimensional molecule is not, however, done as smoothly and simply compared with the building and geometry-minimization routines in ALCHEMY. Standard geometry values are required for the 2D to 3D conversion. These must be checked, and often amended or supplied prior to conversion. The sketch-pad builder is unsuitable for cyclic molecules. The use of templates to build rings is recommended, but it can sometimes be quite confusing as to which atoms in the molecule have 2D coordinates or have been parameterized as 3D. The DELETE ATOM/BOND feature also seems to be unnecessarily complicated; however, with a little more thought all these awkward building features could be greatly simplified. The rotatable torsions are easily modified, and the rotations can be assigned to the functional keys with a programmable step and direction, thus giving a close impression of real-time rotation. The monitoring of chosen interatomic distances can be activated; however, no energy calculations can be performed. A maximum of five molecules can be displayed simultaneously on the screen.

The CRYS-X program can read coordinates from an ASCII file (either fractional or Cartesian), and also output any new structures to a file. It can also prepare input files for the CNDO [16,17] and PLUTO [18] packages, thus providing quite a flexible, easy-to-use interface to these programs. It has a fairly limited fragment library, which can be extended by the user, and structure-building or modification from fragments or by atom addition is simple, requiring a limited knowledge of standard geometry. When adding or renaming single atoms, the type of atom is undefined and must be added through a separate command, a procedure not unlike that of 2D to 3D conversion in CAMSEQ/M. Similarly, the atom types must be added if the ASCII input file contains coordinates only. In such a case the atoms also have to be connected, and this can be done through a command based on a chosen maximum distance. After the type is assigned, hydrogen atoms may easily be added or deleted (or just simply hidden and/or redisplayed). Chiral centres are not recognized by the program, but those recognized by the user can be inverted. An inversion of the whole molecule is also possible. The rotatable torsions can be optimized through sequential step-wise rotations during which the energy (van der Waals and electrostatic) is calculated and reported. (The program is not, however, very clear on how the charges, which must be obtained externally, are read in.) Also, ring structures built within CRYS-X must be optimized externally. Overall it can be said that the building facilities are good, although not as rapid and elegant as in ALCHEMY. CRYS-X caters for 100 atoms; however, the arrays can be expanded depending on the memory available, with the package source code simply being recompiled.

The greatest strength of MOLGRAF is the extensive library of crystal structures of biologically active compounds listed in Tollenaere's 'Atlas of the Three Dimensional Structure of Drugs' [19], and provided with the program. Cartesian/fractional coordinate conversion can be performed. If the geometry is known, a new molecule may be built atom by atom, by modification of the crystal structure, or by editing the existing ASCII file with the molecular structural information. Hydrogens must be added explicitly. A maximum of 200 atoms can be displayed using the Apple II version, and 999 atoms with the IBM version.

The MGP program makes the distinction between non-polymeric and polymeric structures, which then has atoms grouped in so-called residues, i.e., building units of polymer. The coordi-

nates (Cartesian) can be read in from an ASCII file created via an editor. Bonds can be automatically formed, depending on interatomic distanced and atomic radii, and the rotatable torsions can be altered. However, a rather complex set of commands is required in which the atom order numbers (as they appear in the ASCII file) defining the torsion angle must be known. The content of the ASCII coordinate file can be examined interactively, which is absolutely essential in view of how the torsion angles are specified. Modified structures can be written to a file. Since the program does not provide good structure-building facilities (there is an option to display two fragments each in one of the work-spaces and their connection through the append-command; however, this is extremely clumsy), it is a pity that it cannot directly read files in either the Cambridge Crystallographic Data Base [20] or the Brookhaven Protein Data Bank [21] formats. Two structures (a maximum of 600 atoms each) can be displayed simultaneously on the screen. With macromolecules, however, only a specified portion of a molecule (via residue number) can be displayed in each work-space at any one time.

PROMODELER I (another program intended for macromolecules) can read and write data in either the Brookhaven or Konnert-Hendrikson [22] format, or access binary files saved from the previous session. However, the building facilities are rather primitive: one can break or make the bond, but there is no provision for determining the required bondlength; neither is a check provided as to whether the connection made is reasonable on chemical grounds; nor can the molecule be modified by the simple addition or deletion of a single atom. Any residue can be replaced by one chosen from a library (a valuable feature for studying the effect of amino-acid mutation) with conservation of backbone geometry; however, it is difficult to optimize the sidechain position by rotation as there is no provision for continuous distance monitoring. Clashes between atoms can at present only be avoided by visual inspection. A maximum of 5,000 atoms can be displayed with 640 Kbytes of memory, or 2,500 atoms with 512 Kbytes.

3. Structure display

All the programs provide stick models of the structures, colour-coded (except MOLGRAF) according to atom types (or atom labels), which atom labels on or off. All except MGP and MOLGRAF also have the possibility of lateral stereo display. CAMSEQ/M, ALCHEMY and PROMODELER I provide two kinds of stereo, cross-eyed and relaxed, the distance between the left and right images being adjustable in the first two programs. This adjustment is particularly easy in ALCHEMY. CAMSEQ/M, ALCHEMY, MGP and PROMODELER I can also display space-filling models (i.e., VDW surface), with the atomic radii being adjustable in CAMSEQ/M and MGP. MGP also displays shaded ball-and-stick models or shaded ball-and-wedge bonds (which give a spatial impression). MGP contains special features for macromolecules, such as displaying defined slices of the structure, representing each residue as a single ball, and highlighting specific atoms (e.g. backbone) only. CAMSEQ/M has a ball- (all atoms or heteroatoms only) and-stick or wedge-bond display, which also gives a spatial impression, and the option of an ORTEP-type [23] display. Wedge bonds and spheres, scaled according to whether they are near or further away from the observer, are also options in MOLGRAF. This type of display gives a pseudo-3D impression, but the picture can become rather cluttered. ALCHEMY and PROMODELER I provide up-and-down scaling of a structure (i.e., zooming) and positioning of a molecular anywhere on the screen. Upscaling is only possible in MOLGRAF. CAMSEQ/M, CRYS-X, MGP

and MOLGRAF always automatically recentre the molecule to fit the entire drawing region each time a structure is drawn. The best-view option in CRYS-X is very handy, as it reorients the molecule in such a way as to give the best presentation of all atoms, or only those specified. In CAMSEQ/M, ALCHEMY and PROMODELER I, more than two structures can be displayed simultaneously with different colours (in CAMSEQ/M colour-coding works for labels only), and work can be done either on the current (chosen) molecule only, or the whole set. In ALCHEMY this colour-coding is menu-driven and extremely easy to implement. The global or relative rotations and translations are performed by simply clicking the mouse on the rotate or translate scales in ALCHEMY, whereas in CAMSEQ/M this is done by keyboard commands. In PROMODELER I, a cursor-control option where various keys are assigned to manipulative action (e.g., clockwise rotation around an axis, x) is provided. A good impression of real-time rotation can be obtained in all three programs. In MOLGRAF only rotations and not translations, are possible. In CRYS-X the molecule can be rotated around any axis or defined vector. The original view can be easily restored in CAMSEQ/M, ALCHEMY or CRYS-X. These three programs, and MOLGRAF, can also be easily used to measure any interatomic distance, angle or torsion, and to print out this information.

4. Structure comparison

ALCHEMY, CAMSEQ/M, MOLGRAF and CRYS-X can do a rigid superimposition of two structures by a least-squares procedure, matching at least three pairs of corresponding atoms from the structures being compared. The superimposed structures are then redisplayed and the root-mean-square (RMS) of distances (which indicates goodness of fit) reported, except in MOLGRAF. This option, although offered in the documentation of CRYS-X, is not properly described. The superimposition of two structures is possible, but a complicated sequence of commands is necessary. However, there is a working alternative in CRYS-X which provides a 'flexible' fit. Briefly, a set of atom targets is chosen from one structure, then the second structure is called up and a further set of atoms (guides) chosen which are then associated with the first set. The second structure can then be fitted rigidly or flexibly (and the RMS reported) into the guides. In the flexible fit, up to ten torsion angles can be defined which are then minimized using a steepest-descent method. The function being optimized is the weighted (weights are definable) sum of van der Waals energies and distances between atoms in the pairs of guides and targets. A disadvantage of this function is that only the second molecule and chosen atoms from the first are displayed.

Some structural comparison can also be performed in MGP, using its docking command where structures in each of two work-spaces, suitably oriented and in the desired conformation, can be appended to form a single work-space. Distance-monitoring between atoms of the same work-space, or between the two work-spaces, is also possible.

In PROMODELER I, two or more structures can be read in as a single file and then defined as two different subsets. These can be moved independently (using rotate/translate options) so that overlaying or docking of structures is possible. However, apart from visual inspection there is no means of atom-atom association or simple chosen-distance monitoring to provide indications of how to orient molecules with respect to each other.

5. Conformational analysis

Only a very crude conformational analysis can be performed with these PC modelling packages. In ALCHEMY and CRYS-X this involves rigid rotation of rotatable torsions and calculation of the conformational energies (described above). In CRYS-X a step-wise rotation is possible, with the output of potential energy being produced in a histogram form for a single torsion angle. The conformational space can thus be explored taking one torsion at a time. This, of course, is available for non-cyclic torsion angles only. CAMSEQ/M, MGP, PROMODELER I and MOLGRAF offer no conformational energy calculations. It is claimed that CAMSEQ/PC performs a grid-search of the conformational hyperspace for both cyclic and non-cyclic structures, reporting in tabular or graphic form (energy contour maps for any pair of chosen torsions) the local minima, their energies, statistical thermodynamic probabilities, and entropies. It should be possible to include geometrical constraints on these searches and also to include an electrostatic term in the energy potential, as well as a number of other features, which really makes this package appear quite attractive. All this would make CAMSEQ/PC (for any serious work) far more independent of sophisticated modelling packages on a mainframe computer than any of the other modelling programs discussed. Unfortunately, this package has not been made available for evaluation, and it is our experience that features described in the advertising material often fall short of their description.

CONCLUSION

In summary, ALCHEMY is probably the best package for molecule building and display; CRYS-X would be recommended for systems without a mouse and for those with additional programming in mind. Compared to these, the CAMSEQ/M-CAMSEQ/PC combination, although approximately double the price, should make the user less dependent on a mainframe computer, and enable him to do quite extensive conformational analyses. MOLGRAF's only advantage is its extensive library of crystal structures. MGP, although it contains some features specific for the display of macromolecules, can be regarded as the least user-friendly and least suitable for serious work. PROMODELER I, although rather expensive, is a very well-written program and certainly, if more useful features are added in future versions, would be worth consideration; at present it is only suitable for structure display and viewing. It also suffers from the requirement for a PGA graphics card, a rather expensive piece of hardware. The characteristic features of the packages reviewed are summarized in Table 1.

Author's note

There are other molecular-modelling packages available for PCs such as ChemCad [24], Chemmod [25], ChemNote [26], and WAALSURF [27]. However, these programs were not available to us during the course of this review.

TABLE 1
SUMMARY OF COMPARISON OF SOFTWARE PACKAGES

	CRYS-X	ALCHEMY	CAMSEQ/M	MGP[a]	MOLGRAF	PROMODELLER I[a]	COMMENTS
1. Ease of usage							
Documentation	Y	Y	Y	Y	Y	Y	Y = yes, N = no
On-line help	Y	Y	Y*	Y*	N	Y	*Manual essential
Ease of interaction	3	5	5	1	2	5	Score 1–5
2. Structural input							
Fragment library	3	5	4	0	5	0	0 = absence of facility
Building new structure	3	5	4	0	2	0	Score 1–5
Cartesian/fractional conversion	Y	N	Y	0	Y	N	
Ease of geometry modification	5	5	5	2	2	2	
Distance measurement during geometric modification or docking	Y	Y	Y	Y	N	N	
Maximum number of atoms	100*	~1000	~200–300	1200	999	5000	*Easily expandable
3. Structure display							
Stick	Y	Y	Y	Y	Y	Y	
Ball and stick	N	Y	Y	Y	Y	Y	
Space-filling	N	Y	Y	Y	N	Y	
Add/remove H	Y	Y	Y	N	N	Y	
On/off labels	Y	Y	Y	Y	Y	Y	
Colour coding	Y	Y	Y	Y	N	Y	
Stereo	Y	Y*	Y*	Y	N	Y*	*Relaxed and cross-eyed stereo
Manipulation in 3D space	3	5	5	2	1	5	

4. Structure comparison							
Rigid superimposition	Y	Y	Y	Y	N	Y	
Flexible superimposition	Y	N	N	N	N	N	
5. Conformational analysis							
Potential-energy calculation	Y	Y	N	N	N	N	
Structure minimization	N	Y	N	N	N	N	
6. Miscellaneous							
Source code	Y	N	N	N	N	N	
No. of interfaces to other programs	2	1	3	0	0	2	
Graphics card required	EGA/CGA	EGA	EGA/CGA*	EGA	EGA	PGA	*Hercules also available
Mouse option	N	Y	Y	Y	N	Y	
Price ($US)	<500	<500	<1000	<500	<500	<1000	

[a]These programs are intended for use with macromolecules

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