

Structure Drawing and Molecular Mechanics Programs.

Jim Beatty

Programs to draw structures and manipulate them are many. This listing includes only those I have literature for. There are more on the market. Upgrades are constantly being made. Prices quoted are for single academic copies. Most suppliers will send you a demonstration disk for a small charge or no charge. Some suppliers will send you programs on an approval basis. Some include minimization programs such as MM2, while for others you must purchase the program separately.

I consider these programs as word processing programs for chemical structures and more. I believe that one or more should be available to undergraduate chemistry students.

I. Tripos Associates, 1699 South Hanley Road, Suite 303, St. Louis, MO 63144-2913. Phone 800-323-2960.

Alchemey III, a powerful molecular modeling program for IBM compatibles or Macintosh computers. Prices start at about \$500. MM2 available for IBM machines for \$200.

LabVision, an advanced molecular modeling program for computer workstations. \$2500. 30 day free evaluation available.

II. Serena Software P.O. Box 3076, Bloomington, IN 47402-3076, Phone 812-333-08232.

PCMODEL Molecular modeling for all worlds. Prices start at \$200 and go up to about \$4000 for programs for the fastest workstations.

III. Trinity Software P.O. Box 960, Campton, NH 03223, Phone 800-352-1282.

CHEMWINDOW, CHEMINTOSH and CHEMDRAFT III are basically structure drawing programs. CHEMDRAFT in version III has grown into a 3-D molecular modeling and presentation graphics program. Prices start at \$99.

IV. Oxford University Press, 200 Madison Avenue, NY, NY 10016, Phone 212-679-7300.

Desktop Molecular Modeller for the IBM PS/2 55 compatible or above. A powerful and interesting molecular structures program which has a number of interesting options including a symmetry operator program for inorganic structures. Prices start at \$495.

V. Springer-Verlag New York, Inc., Electronic Media Department, 175 Fifth Avenue, New York, NY 10010, Phone 212-460-1653.

Moby is an interesting molecular modeling program for the IBM PC or compatible. Some very interesting options. Prices start at \$498.

THE USE OF LINEAR LEAST SQUARES IN UNDERGRADUATE CHEMISTRY LABORATORY COURSES

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INTRODUCTION

The availability of micro-computers and appropriate software make the use of numerical and statistical methods by undergraduates readily feasible. The important question is how useful and meaningful is the use of such software by undergraduates? There is a risk that either too little or too much information about a numerical or statistical method is provided to the student. If too little information is provided, the student goes through a process which provides some computer output, but obtains no real understanding of what the information obtained means and how it is to be used. If too much information is provided, the student may become confused and frustrated. The level of instruction must be appropriate, considering the abilities and needs of the students.

Linear least squares is one of the most useful statistical methods for beginning students. In the pre-computer days it was common to include an experiment in the junior or senior level physical chemistry or instrumental analysis laboratory course which involved a linear least squares calculation. This exposed the student to the technique. Because of the amount of time required to do the calculations either by hand or calculator, it wasn't really feasible to have the student carry out more than one or a few least squares fits.

At Clarkson where every student has a computer (currently an IBM PS/2) in his (or her) own room and where there are computers in the laboratory and elsewhere on campus, I have asked students to use linear least squares software in a second semester freshman laboratory course and a second semester junior combined analytical - physical chemistry laboratory course.

In this article I will describe how linear least squares can be introduced at an elementary level. In my view it is not essential that