COMPUTER SOFTWARE REVIEWS

CHEMiCALC. The Chemistry Companion

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CHEMiCALC[1] is designed to be an aide in the teaching and learning of basic chemical calculations. The MS-DOS package reviewed here consists of the software and a 107-page Companion Guide to Problem Solving. The system requirements to run CHEMiCALC are minimal. The specific machine used for this evaluation was an IBM PS/2 Model 30/286 without the optional CHEMiCALC TouchPad. A second implementation of CHEMiCALC, a handheld calculator, is also being considered.

The six computational modes available are ELEMent, PAIR, FORMula, CALCulation, RXN(Reaction), and EMPirical formula. Context-sensitive help is always available. ELEMent mode is used to display a variety of physical properties for a specified element such as atomic mass, boiling and melting points, electronegativity, and specific heat. There are also options for graphically displaying a property in comparison to other elements on the Periodic Table. The graphs dramatically show the trends in physical properties. PAIR mode is used to do pairwise comparisons of properties of elements in a compound such as electronegativity difference and ionic and covalent internuclear distances. FORMula mode is used to calculate molar mass and percent composition. CALCulation mode is used to complete mole-to-mole, mass–mole calculations for a compound and unit conversions. RXN(Reaction) mode is used to write and balance reaction equations and to complete stoichiometric calculations based on a reaction equation. EMPirical formula mode is used to complete computations involving percent composition information and empirical and molecular formulas.

The Companion Guide to Problem Solving is written to be both a user's manual for the software and a tutorial in stoichiometric calculations. The reader is first given instructions on the use of the keyboard and then exercises for each of the six computational modes available within CHEMiCALC. Often, an exercise is divided into two parts. In the first part, a sample calculation is broken into a series of steps and completed as if it were being done by hand. In the second part, the key strokes are given for doing the same calculation using CHEMiCALC with representations of CHEMiCALC's display for that calculation. This side-by-side approach is helpful, except when there are errors in the Guide or the representations in the Guide do not match the actual display. All the discrepancies noted during the evaluation involved errors in the Guide, and some are easy to detect. In one problem, the instructions for using the TouchPad and keyboard did not involve the same numbers. In another, there is an error converting grams to milligrams.

However, it will not always be easy for a student to decide whether there is an error in the Guide or an incorrect key stroke has been made to CHEMiCALC. The representation in the Guide of the graphical comparison of the density of the halogens does not match the actual screen display. The values in the Guide for the density of fluorine and chlorine are incorrect. To complicate matters, this comparison is potentially confusing because density values for two gases, a liquid and a solid, are displayed on the same graph.

It is hard to evaluate this package without considering its impact on students and student learning. To begin, I would not recommend asking students to use CHEMiCALC without the optional TouchPad. With regular use, the key strokes would likely come almost automatically. However, I suspect a student would find it difficult to master simultaneously both the chemistry and the key stroke combinations.

It is also not obvious how CHEMiCALC will enhance learning because it provides answers to most calculations with little input from the student-user. For example, all the student-user need do in FORMula mode to obtain the molar mass and percent composition of a compound is enter the formula. The student-user is not prompted to enter their own estimates.

In RXN(Reaction) mode, there are two ways to balance an equation. The equation balancer can be used to balance the reaction starting with one entered as the coefficient for all products or reactants. Equations balancer – check, can be used to check for balance using coefficients entered by the user. Unfortunately, the equation balancer can be invoked immediately after all the formulas have been entered. There is nothing to force the student-user to enter their own coefficients before using the equation balancer.

Also, it is possible to write and balance ionic equations in RXN(Reaction) mode. The example worked in The Chemistry Companion involves the reduction of dichromate ion in acid with tin(II). Unfortunately the fact that this reaction involves oxidation–reduction is masked in the balancing process. There does not appear to be a way to either show the electrons transferred between the oxidation–reduction processes or independently balance the half-reactions. Finally, the charges on the ions are not displayed with the final, balanced equation.

In PAIR mode, CHEMiCALC dutifully displayed the electronegativity difference between krypton and xenon, an estimated value for the percent ionic character in a bond, and covalent and ionic internuclear distances. It might have been pedagogically sound to at least question if I had meant to enter that pair of elements because the probability of forming such a compound is small.

I would suggest that persons interested in CHEMiCALC compare it to software that requires the student-user to be more active in the problem solving process and provides more evaluation and feedback. Examples of this approach would be Volumes I and II of TOOLS OF CHEMISTRY.[2]

During the evaluation, a major problem was discovered in CHEMiCALC. Dr. Bert Ramsay, the author of CHEMi-

CALC, answered the telephone at Chemical Concepts Corp., listened to my questions and comments, and had a new version with the problem fixed to me in less than a week. He also included a draft copy of a second pamphlet being written for users of the package. It is a case study of a typical first year chemistry problem, demonstrating common student errors and how CHEMiCALC might be used to assist a student.

Dr. Ramsay is very concerned with creating a sound product and, to that end, is having it tested in high schools in Michigan. I will be very curious to learn the outcome of that testing, particularly if there is any demonstrable improvement in learning. However, given the errors detected in the Guide and the cost of providing enough software packages and TouchPads for a laboratory, I would be hesitant about buying CHEMiCALC until improvement in learning can be shown.

REFERENCES AND NOTES

(1) CHEMiCALC is produced by Chemical Concepts Corp. 912 North Main St., Ann Arbor, MI 48104. The list price of the basic software package for MS-DOS machines is $129. An optional CHEMiCALC TouchPad is available for $199 plus the cost of an appropriate interface ($15–375).

(2) TOOLS OF CHEMISTRY is written by John Weyh, Joseph Crook, and Les Hauge, of Western Washington University, and distributed by Trinity Software, P. O. Box 960, Campton, NH 03223.