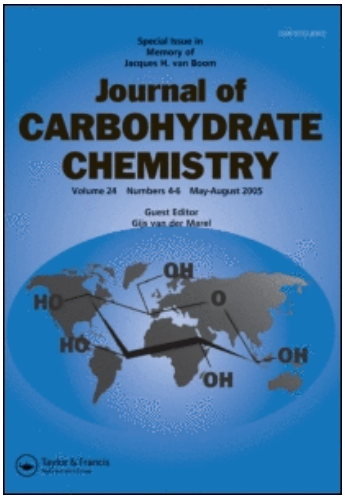

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Software Review

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SOFTWARE REVIEW

CHEMCAL. By R. A. Wertz and W. T. Brinkley. B & B Scientific Software. Phoenix. 1985. $89.95.[1]

The CHEMCAL program is a new, user-friendly software package for the IBM-PC or Apple II microcomputer marketed by B & B Scientific Software for the calculation of elemental percentages in organic molecules. The package contains four programs: README, PROG1, START, and FORM10. Only two of these programs are accessible to the user, README and START.

START is the program for the calculation of elemental percentages. This menu-driven program consists of four sub-programs: Program A: Mole Formula to %; Program B: % to Mole Formula; Program C: Elemental Ratio; and Program D: Atomic Weight Table. Program A steps through all the supported elements and provides an opportunity for verification. The result of the input is then provided along with four options: RETURN TO SMALLEST RATIO, MOIETY ADDITION/SUBTRACTION, SOLVENT ADDITION/SUBTRACTION, and MAIN MENU, all of which are self-explanatory.

Program B converts the experimentally determined compositional percentage to the molecular formula in terms of the smallest ratio of supported elements. Multiplication of this ratio can easily be processed if desired. The minimum oxygen percentage required for this program is 1.125; if it is less than 1.125, then Program C should be used.

A Table of Atomic Weights in Program D provides the atomic weights of the first 93 elements based on the 1983 IUPAC values.

The reviewers found this calculation package to be extremely easy to use and efficient in its calculations. The straightforward explanations provided in the concise, yet informative manual enables one to perform calculations expeditiously. Program A was found to be most beneficial, especially with regard to the added features of moiety or solvent addition/subtraction, a feature especially helpful to carbohydrate chemists who frequently encounter hydrates or solvates. Supported solvents are water, DMSO, ethanol, methanol, chloroform, THF, dichloromethane, ether, and acetonitrile. These may be added in any increment, either as single mole fractions or in specified ranges of four at a time. Five unassigned slots allow one to add solvents to the program as needed. The addition of a moiety or solvent at specified increments enables one to quickly verify experimentally determined elemental percentages.

One drawback of this software package is the somewhat troublesome addition of elements to the dataset that are not

included in the supported element set. (Supported Elements: C, H, N, S, P, F, I, Br, Cl, and O) Silicon, as an example of a frequently encountered element, must be entered as a fraction of a supported element (e.g., 0.8760S or 0.9068P, etc.) An 80-element version of the program is under development for those with frequent demands for additional elements.

Both IBM-PC and Apple IIe versions were evaluated on machines having 640 and 64 Kb of memory, respectively. Calculations were virtually instantaneous on the former, but yet impressively fast on the Apple. The Apple version lacks the screen-dump print feature that is functional on the IBM-PC version.

Overall, the CHEMCAL software package would be a good addition to the software library of an individual chemist or group of chemists who require elemental percentage calculations on a regular basis.

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[1] Orders may be placed with: B & B Scientific Software, 1124 East Portland Street, Phoenix, AZ 85004. Phone: (602)254-8377. Specify computer when ordering. The program will run on an

IBM-PC or compatible computer using DOS 2. or higher, with 128 Kb, minimum, or on an Apple II+ or IIe with DOS 3.3 and an 80-column card.