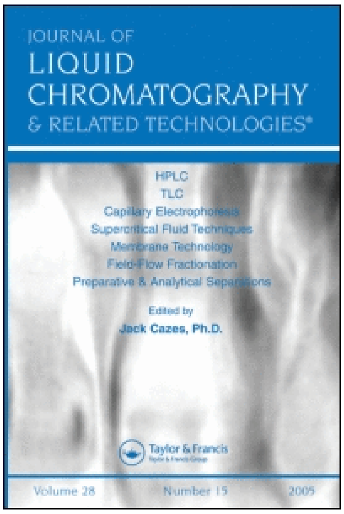

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A review of "Introduction to Organic Chemistry, An American Chemical Society Computer Course, Stanley G. Smith (Univ. of Illinois), Compress O i v ., Van Nostrand Reinhold Co., Inc., Wentworth, NH, 8 diskettes, $375.00 (US)"

J. A. Kuck[a]
[a] Fairfield University, Fairfield, CT

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BOOK REVIEW

INTRODUCTION TO ORGANIC CHEMISTRY, An American Chemical Society Computer Course, Stanley G. Smith (Univ. of Illinois), Compress Div., Van Nostrand Reinhold Co., Inc., Wentworth, NH, 8 diskettes, $375.00 (US).

As one who has been associated with the learning and teaching of organic chemistry at various levels for more than half a century, this reviewer accepted his invititation with great interest and expectation. He was not disappointed; the computer program under review is quite fascinating. There were seven discs to examine; (the eighth was a chemistry game which the reviewer did not see.) But the seven under review comprised the following: 1) Alkanes and Alkenes, 2) Substitution Reactions, 3) IR and NMR Spectroscopy, 4) Arenes, 5) Alcohols, 6) Aldehydes and Ketones, and 7) Carboxylic Acids.

This interesting set of computer lessons is advertised to the student in the introduction of Disc-1 as "A short course in organic chemistry which is suitable for home study or as a supplement to a college level course." However, after having worked our way through the whole program, we are inclined to question the validity of the first claim on several grounds. First, -- we noticed that many questions were asked of the student operator that he could hardly be expected to answer without previous knowledge acquired either in a classroom or from reading a good text. Furthermore, although the list of the seven topics treated seems quite impressive at first glance, a more sober reappraisal of the list as it presently stands, soon brings one to realize *that if this is all there is, the list is far too short for even a "short* course" in organic chemistry. In fact, the program as presently constituted cannot possibly give the student a bird's-eye view of the field. For the material presented, while intrinsically good in itself, may be likened, as it were, to but a few bold strokes of the artist's brush at the start of an immense canvas.

Consequently, the second claim for the usefulness of the program as a supplement to a college level course in organic chemistry is more to the point. By virtue of its numerous challenging questions and problems, the program can serve as a tough drill-master for the under-achiever, albeit an expensive one. Then, too, successful completion of such a rigorous series is bound to give the timid student a feeling of self-confidence. This is good.

In the following remarks this reviewer has tried to confine his criticism to broad general considerations of importance and, in order to save space, has overlooked many small points where he could personally disagree.

Disc-1 starts out with the Lewis dot diagram for methane. Unfortunately there is no symbolism to distinguish the electrons belonging to one element from those belonging to the other. Nevertheless, such custom is good for the student at the start and can be quite useful later on with more complex structures. The author does well to emphasize the stereochemistry of methane right away and his use of the wedge and dotted line as a conceit for valence bonds extending in front of or behind the plane of the screen is worthwhile.

Groups of student practice problems appear on Disc-1 and crop up every so often throughout the whole computer program. Where an organic structure has to be supplied by the student operator in answer to a request for a reaction product or starting material, the computer offers him a small group of number-coded building blocks from which to assemble his desired molecule. For example,"0" stands for a quaternary C, "1" for a CH, "2" for a CH_2, "3" for a CH_3, and other numerals on occasion for CO, OH, NH_2, Cl, Br, etc. If the student punches in the proper digits (and only in the correct order), the completed structure will appear on the screen as it is built up bit by bit. The student then receives an accolade for his successful effort.

It is this reviewer's experience over many years of teaching, that students learn organic chemistry best by writing structural formulas from dawn to dusk. Hence, we deliberated at some length whether the present computer system was really in the student's best interest. Would it not be better for him to be doing the same work at the blackboard? However, we finally concluded that the psychological process is probably about the same in both situations -- the only difference being that at the blackboard the student has to write out all of the hydrogens himself and check each carbon for its proper valence. Whereas with the computer, the hydrogen count and the tetravalency of carbon are automatically taken care of for him; thus he is relieved of such responsibility and this may not be good for him.

Continuing on in Disc-1 we come to the development of the stereochemical structure of ethylene. Here we think that the author has taken too much for granted. Also, he has confused atomic orbitals with molecular ones. (He has made no previous mention of Pauling's hybridization (sp^3mixing), an important assumption for the 109° 28'' valence angle in methane.) The computer merely tells us "Carbon has an s and three p orbitals in the valence shell. These orbitals may be used to make up to four bonds to carbon. We will use one s and two p-orbitals to form the sigma framework for ethylene." It does not say that two carbons, each with its own s and its three p orbitals, can each form three hybridized sp^2 atomic orbitals from two of the p's with the one p orbital remaining unhybridized. Nor that the three hybridized sp^2 atomic orbitals on each carbon can form three molecular orbitals with each of the two hydrogens and the adjacent carbon.

Next, there flashes before us a sketch of ethylene in three dimensions. But there are only two leaders labeled "σ-bond" instead of three, thus detracting from a complete explanation here.

The point is that this section deals with very tricky materials. A careful, explicit explanation is required at this point if the student is to see the whole picture.

Disc-2, The Mechanism of Substitution Reactions, is very well done. By means of animation and graphics the author illustrates very neatly the kinetics of the reaction between MeBr and NaOEt. The concepts of the rate constant and the transition state are clearly presented along with the parameters of concentration and temperature in the rate equation.

An interesting racemization and exchange experiment has also been stored on this same disc. Monodeuterated benzyl bromide is reacted with lithium bromide to investigate its loss of optical activity with respect to the concentration of LiBr. An automated backside displacement portrays the inversion of configuration and clinches the mechanism of S_N2. Then the bimolecular nucleophilic substitution mechanism is further emphasized in the tosylation of a 2-butanol enantiomer followed by an inversion reaction with KOAc. Subsequent hydrolysis of the resulting ester yields the opposite form of the original alcohol.

Disc-3, IR and NMR Spectroscopy is an effort by the author to introduce the student to these valuable experimental techniques. The simple physics of each operation is first described; then problems to identify various structures through interpretation of their two kinds of spectra are posed to the student. This reviewer feels that this section can present more frustration to some students than any other part of the series. With the NMR particularly, more and better explanation of the characteristic peaks and spin-spin splittings for certain structures and functional groups, with examples, ought to have been provided before asking the student to interpret unidentified spectra. For without sufficienttraining beforehand, impatient students may be expected to gamble blindly with guesses as if the computer were a slot machine. Also, under basic NMR theory when listing the magnetically susceptible atomic nuclei ^{1}H, ^{13}C and ^{19}F, the author inadvertently omitted ^{31}P. The latter is perhaps more important than ^{19}F. Nevertheless, the combined IR and NMR problems presented at the end of Disc-3 are good in spite of their difficulty.

Incidentally, the author in defining the IR spectrum as a plot of absorption vs. frequency ought to have introduced the term "Wave number" for cm^{-1} at the start. At present, this term suddenly appears without comment much later on.

Disc-4, Arenes, begins with a consideration of the structure of benzene. Here we were unhappy with the author's sketchy treatment of the problem. For without any preliminary explanation, the student is shown a side view of a hexagon consisting of six carbons, apparently trivalent, and is asked "Is the hybridization of carbon sp, sp^2 or sp^3? (meaning: "In this particular structure and not in methane or acetylene.") Then if he makes the wrong guess, he is told "There are three bonds to carbon so type "2" (i.e. for sp^2). (Careful instruction about hybridization is needed beforehand; it should have been given back on Disc-1, but was not!) Next, the student is asked "Is the remaining orbital on carbon s or p?" Whereupon the surface of the p-orbital suddenly appears and he is told "Sidewise overlap of these p orbitals gives a Π-bond above and below the plane of the ring." But two arrow heads and leaders each labeled "Π-bond" and pointing to upper and lower dotted lines suggest to engineers that there are indeed two Π-bonds, one above and the other below. This, of course, is not so.

Finally, the student is shown Kekulé I ↔ Kekulé II as an alternate representation of benzene and the show is over.

How much better would it have been to have started out with Kekulé in the first place and then explain that the idea of the resonance hybrid has been superseded to some extent by today's application of the superior orbital theory.

A little further on in a comparison of the heats of hydrogenation of cyclohexene, cyclohexadiene and benzene the student is given the ΔH's for the first two reactions and is then asked "Would you expect hydrogenation of benzene to produce more or less heat than cyclohexadiene?" Of course the uninformed student logically expects "more", but when he says so, he is told "Type: less". (Serious students sometimes resent what they consider to be unfair entrapment and have less respect for the entrapper.)

Before leaving Disc-4 we should not forget to mention that the theory of directive influence (orientation effects) is well presented. (Unfortunately, when NH_2 was listed in the group of o, p directors, no mention was made of the techniques for "protecting" groups from the action of antithetical reagents. While discussing the directive influence of NH_2 this is a good place to introduce the topic.)

Discs-5 and 6, Alcohols; Aldehydes and Ketones must be lightly reviewed here on account of limitation of space. Suffice it to say, that their organic chemistry is straightforward and conventional. Eighteen practice problems involving use of the Grignard reagent are given under "Alcohols" and fifteen exercises in carbonyl chemistry are presented. Included in the latter are several that compare the relative merits of $LiAlH_4$ and $NaBH_4$ as reducing agents. Important reaction mechanisms are also explained and everything is well done.

Disc-7, Carboxylic Acids, however, was more of a problem for the reviewer. Several serious errors in the esterification experiment were spotted and have to be reported. First, in the graphic demonstration when the buret reading is found to be 17.5 ml, the student is told: "This is the initial acetic acid titer." Unfortunately, this is an absolutely incorrect use of the term "titer" and is an error that many chemists commonly make. The "titer" is a volumetric chemical factor; not a volume measurement.*

Next, we have to point out that the computer sketch of the esterification set-up is bad. Heating an esterification mixture in an unprotected R.B. flask over an open flame is an unsafe practice today. It is to be condemned.

Finally, the calculation of the equilibrium constant is incorrectly set up. The author starts out with the reaction products and reactants in their respective brackets which mean "moles/liter". Nothing wrong yet! However, he continues with the explanation: "You titrated a 1-ml sample with 0.5 M NaOH. Therefore, the concentrations are:

Initial = 0.5 M x 17.5 ml/1 ml = 8.7 M
Equilibrium = 0.5 M x 6.6 ml/1 ml = 3.2 M "

Since "M" denotes "moles/liter", the 8.7 and 3.2 here are absolutely wrong! A quick computation shows the initial amount of acetic acid present to be 8.75×10^{-3} moles. In order to determine the actual concentration we have to know the volume of solution which we can estimate from the densities of the two reactants. The total starting volume thus comes to about 57.7 mL. Assuming that only two 1-ml aliquots of reaction mixture had to be withdrawn (i.e. at 0 min and 60 min respectively) the volume becomes 55.7 mL. The

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* "Elementary Quantitative Analysis" by W.J. Blaedel & V.W. Meloche, 2nd Ed., p.238, Harper and Row, New York, 1963

initial concentrations of HOAc and EtOH come out to be 5.05×10^{-4} M (not 8.7 as stated). Likewise their final concentrations at equilibrium prove to be 5.7×10^{-2} M (not 3.2M). For the concentrations of EtOAc and H_2O present at equilibrium the figure is 1.005×10^{-1}M (not 3.1 M). Inserting the correct concentration figures into the equilibrium equation yields a k value of 3.16.

How could the author have gotten the correct value for k with his faulty use of the symbol M? The answer is "by a compensation of mathematical errors!" (The volume figures (55×10^{-3}L) in the concentration denominators and the exponent factors (10^{-3}) in the numerators all cancelled out giving him the proper value for k.) However, just because the author got the right value for k does not excuse his original statement of "AcOH Initial = 8.7 M Final = 3.1M." Grizzled analytical chemists call the use of such "working calculations", i.e. abbreviated mathematical formulas known to give the right answer by experience, "evasive thinking". It is not good for the student and may tend to confuse him.

This reviewer would close, however, on a more positive note. It is obvious that the present computer program has many good things to be said for it. It is a pioneering attempt to teach organic chemistry in a quick and easy fashion using the time-honored art of Socrates which works. Also, the computer with its animated illustrations and graphics combined with instant calculations has a powerful advantage over a book.

The author has been quick to seize upon this. For example, he has used animation very effectively to demonstrate various reaction mechanisms like those of catalytic hydrogenation, the addition of HBr to unsymmetrical olefins, backward displacement, and ester hydrolysis -- to mention only a few. His use of animated rotation to illustrate conformational analysis for the ethane molecule is a mnemonic success.

Also, in the esterification experiment, for example, the computer's ability to graph the mathematical function over a range for any value of the independent variable to be chosen by the student himself is truly captivating! All of this makes for fun and can convert the learning process into a fascinating game -- the eternal goal of all good teachers.

But, in this connection, the reader is referred to a recent article that appeared in Science* entitled "Will Home Computers Transform Schools?" Teachers and software makers say "Yes", but problems of equity and quality of course work remain unsolved. If it is true that 80% of the educational programs have gone on the market with little or no research or testing, the present program is in great contrast on account of its high quality.

"Introduction to Organic Chemistry" is a significant step forward. It is an easy computer program to operate. It will undoubtedly be expanded in the future beyond our imagination. Although it is already an achievement, the present accomplishment is only a challenge for the author and others for the computer Beilstein and text of the future. "What comes from acorns?" "Type: oaks".

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*Science: 20 July 1984, No. 4659, p.296.

J. A. Kuck
Fairfield University
Fairfield, CT