THE EDUCATIONAL FOUNDATION OF COMPUTATIONAL CHEMISTRY

It is probably fair to state that Computational Chemistry is becoming a field unto itself, in the same sense that Analytical Chemistry has become a 'field' of chemistry. Both Computational Chemistry and Analytical Chemistry must be prepared to work across the broad spectrum of chemical problems which characterize today's chemistry. Neither, for example, has the luxury of working on organic molecules alone.

Despite the similarities one can cite, there is one important difference between these fields. Analytical Chemistry has, underpinning it, an accepted educational foundation — a foundation which Computational Chemistry does not enjoy...as yet. To be sure embryonic efforts at developing such an educational base are taking place, often in some of the least expected locales.

QCPE communicates with thousands of people in the course of a year. We are aware of many educational developments (although by no means all, perhaps not even the majority, of them). Still, in almost any university or college today, there appears to be someone who is attempting to introduce the ideas of Computational Chemistry into the established chemistry curriculum. The mode of introduction may be a new course or the modification of an existing one. What is perhaps most surprising is that much of the effort is manifesting itself in small, often private, schools.

Almost a decade ago, Reed College in Portland, Oregon, systematically set up a program (as best as one could be defined at the time) in Computational Chemistry. Small schools — Bard College in New York comes readily to mind — have been developing programs for several years now.

QCPE is constantly being asked about any advice that might be available about organizing such a program, and we note that most of these inquiries emanate from the small, private schools — the type of schools that are hiring faculty whose principal responsibility is to establish and refine such programs.

With a certain bemusement, we also note that the chemistry departments in our major universities are behaving as if nothing has changed. For them, what was chemistry yesterday will continue to be chemistry into the foreseeable future. One cannot help but be reminded of the Titanic sailing blissfully toward her rendezvous with the iceberg....

One is forced to ask the question: WHY?—what differentiates 'major' universities from small colleges in terms of educating undergraduate chemists? What opportunities do small schools see that major schools fail to recognize—or perhaps refuse to acknowledge? Over the years, QCPE has carried out a sort of informal survey to address such questions. Many may find the answers surprising.

Obviously, a major difference lies in the area of available resources. The practice and teaching of chemistry is a very costly undertaking—so costly, today, that experimental chemistry as a technique may only be available to schools whose endowments can absorb the costs of extensive programs. Interestingly enough, experimental chemistry teaching laboratories have become so expensive to operate that even major universities are looking for ways to economize. But they still

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attempt to convey the body of knowledge which is chemistry in an essentially experimental (read: traditional) mode.

The smaller schools are equally dedicated to doing as good a job as possible in the teaching of chemistry. They simply recognized early on that they lacked the resources to compete directly with the major schools. Thus they have systematically been trying to exploit Computational Chemistry as an economically viable alternative to the traditional experimental approach. Their attempts certainly merit a second glance.

Experience has demonstrated that, properly exploited, the techniques of Computational Chemistry can indeed provide the student with a valid and substantial understanding of chemistry. It does not provide it in the identical context, perhaps, but it may provide a more thorough understanding in a much shorter time.

The hardware required for this type of education is no more expensive than many of the microcomputers now broadly available and well within the reach of even the smallest schools. The software for these computers is readily available. The microcomputer has, in its own way, become the 'great equalizer' between the large university and the small college. In short, the large school, by virtue of just being large, does not really have all that great an advantage!

As often as not, the people at these smaller schools who are taking the responsibility for forming Computational Chemistry programs are not, at the outset, all that broadly knowledgeable about the field. Their backgrounds are varied, but they do tend to reflect some involvement in computer usage. With the acceptance of the responsibility, however, these people typically tend to develop rapidly, because of the nature of the field—perspective develops quite quickly.

The use of computers as a means of preparing tomorrow's chemists is an enterprise still in the early stages of its evolution. The computational tools are now in place; however, the exploitation of these tools will depend on adequate graphics—especially in an educational situation. Fortunately, graphics as a field is probably more advanced on microcomputers than on mainframes, so we are now positioned to do the job properly.

Our conclusion is simple: A strong educational foundation for Computational Chemistry is being laid. Although the leadership has arisen from an unexpected source, it is, nevertheless, there. Perhaps this 'grass roots' approach will only stengthen the ultimate educational response to the field.

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