THE BEST OF TIMES AND THE WORST OF TIMES

It has become clear to even someone who is not a professional economist that we live in 'interesting times'. All over the industrialized world we hear stories of restructuring and downscaling. These are, of course, polite words for unemployment. Middle managers, are being removed in large numbers as it has been discovered that these people are mostly information facilitators, and the dread threat of the impact of computers on society is finally beginning to be realized in these echelons of workers. Computers are replacing human beings in these situations.

The research community is also not being spared from these rearrangements in the way work is to be accomplished. In both the United States and Europe, and to a lesser extent in Japan, stories are beginning to emerge of massive layoffs in the chemistry research community. In the United States, the petroleum industry appears to be the most thorough example of this practice, and the reasons are not clear as to why it is going on.

On the basis of the economic fundamentals now in place, there is little justification for these actions. The sorts of reductions in the workforce which are now being seen indicate that many organizations are simply not going to be doing any research for at least the next three to four years. They must be operating under the assumption that their need for research and new products will be minimal for this period. They must, therefore, be preparing for a long period of economic stagnation.

If one looks objectively at the cost of doing research in chemistry these days, it can be easily understood that a vast amount of scarce capital can be saved simply by not doing this research. 'Wet' chemistry is now terribly expensive. As long as one's competitors are in the same situation there is no threat to market share in standing down for a few years. But herein lies a major assumption.

Let us suppose for a moment that one's competitors stop doing wet chemistry along with everyone else, but quietly switch to investigating what can be done with computational chemistry. Let us also suppose that they begin to develop a certain expertise with using the many computational tools now available to advance their research and begin to enhance their existing product lines at first and even break new ground with potential future products.

In the beginning the process would move slowly. Most research groups approach their work in a similar manner. The way they do research is dictated by the instrumentation they have available and the research techniques with which they are familiar. When beginning to use computational chemistry, they would be learning an entirely new approach to asking questions and they would also be learning the capabilities of a completely new set of tools. They would need to establish the limits of each tool and the appropriate areas of application.

A major advantage of computational chemistry which very few people are aware of is that the learning curve is very steep (i.e. fast). With a minor amount of outside assistance, experimental chemists can become very adept at using computational tools. This has been seen frequently. There is such a vast array of tools available that it would not be necessary for any research organization to have to develop its own tools at first. Great strides could be made with just the tools that are available.

Eventually, our hypothetical research organization would come to rely on computational

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chemistry to a yet greater degree. The cost of wet chemistry would no longer be a major consideration as they would be doing only a limited amount of it, and this work would be highly focused. What would ultimately emerge would be a research paradigm which would permit the rapid and inexpensive development of new products. These products would begin to appear in significant numbers and they would catch their competitors in a very vulnerable situation. It could well be the case that the competition would be in no position to ever recover the lead which had been lost in terms of both research costs and market share. It could be the beginninig of the end of well-known companies. When a paradigm changes, many older firms simply go away. We are clearly in a time of great change.

I have developed this simple parable to bring to everyone's attention a situation which provides a major opportunity. It is expensive to do wet chemistry. At the moment, we work in constrained economic times. We need not, however, forsake the many benefits which mankind can derive from the practice of chemistry because of the times. By making a careful transition from an almost total dependence on traditional chemistry to a situation in which we obtain computationally as much information as we possibly can, we should be able to move forward and perhaps even advance in our use of chemistry. We need to make a change of paradigm.

For those people who now work in the field of computational chemistry, these times must be viewed as the greatest opportunity to exploit their training and experience. These times present one with an opportunity to step forward and demonstrate the leadership which could benefit not only one's employer but our society at large. For those research organizations which remain firmly rooted in what I will refer to as traditional chemistry, these could also be perilous times which many companies may not survive. We are at a turning point, at which the few may flourish and the many will be lost. This is the sort of situation which Dickens surely had in mind when he wrote: 'It was the best of times, it was the worst of times.'

Richard W. Counts
QCPE
Indiana University
Bloomington, IN 47405
U.S.A.