FORGING THE FUTURE

Computational chemistry finds itself enmeshed in a revolution. Modern technology has yielded computers which can sit on one's desk and provide the individual with more computing power than was hitherto available from a central computing facility. All this in barely two decades; yet, despite these advances, we are not yet quite able to practice computational chemistry on the scale we are able to envision it.

In previous columns, we attempted to focus on the strengths and weaknesses of the various computational methods available to us. From this beginning, we are able to conclude that there are many problems of chemical interest which we simply cannot attack in a completely satisfying manner.

Some people seem to be of the opinion that all we *really* need are considerably more powerful computers — the 'if only we had computers a hundred or perhaps a thousand times more powerful, we could attack any problem' school of thought. Clearly, the enhancement of computer power over the last decade leads one to expect further such strides in the future. Despite this possibility, however, many of us have the gnawing suspicion that this purely technological solution is too simplistic.

Even with a thousandfold increase in computing power, for instance, we obviously could not blindly apply Ab Initio techniques to any and all conceivable problems. These techniques are the most general (from a conceptual viewpoint) but would unlikely be able to calculate structures to the accuracy of Molecular Mechanics, especially if transition metals were involved. In short, no matter the computing power, the current Ab Initio techniques are just not suitable for an effortless, black-box approach to everyday chemistry questions.

Molecular Mechanics, of the Allinger variety, is perfectly capable of yielding highly precise structures — if only those critical force-field parameters were available. There is always a caveat — and here we are faced with a big one, i.e., we have very few of these desperately needed parameters available to us. In a 'best of all possible worlds' scenario, in which parameters for all components of the Allinger force field, covering all major chemical elements, were available, *then* a thousandfold increase in computer power would provide the tool to permit us, essentially, to 'engineer' solutions to molecular questions. But (another caveat) we would still need to make some use of techniques to produce a wave function to permit us to lay this critical information over the structure Molecular Mechanics has given us.

As always, we stand before infinite questions with but finite means (resources). As a result, we are forced to focus our energies so that we may obtain maximum effect from these limited resources.

This sort of analysis is not new. Many other groups have wrestled with these problems. The judgment that has emerged, virtually a consensus, is that first and foremost we should bend our efforts toward obtaining the critical force-field parameters for Molecular Mechanics. I concur.

To this end, several groups have coalesced to investigate ways and means to reach this goal. A prominent effort in the United States, for example, has focused on calculating these parameters by

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working with small molecules and extracting the parameters from Ab Initio calculations. Such an approach is slow and costly — and the parameters obtained will be no more accurate than current Ab Initio techniques permit them to be. Still, they will have been obtained in a logically consistent manner and certainly should extend the range of problems which can be confronted.

Uncounted others — individuals and groups — are simply making up and testing parameters, which are often being used internally by large corporations and are even making their way into the literature. But one has no safe way to judge their value; there is grave potential danger inherent in assuming the general validity of parameters so obtained.

Recently, Jeffrey M. Wales of Polygen Corporation proposed that we (interested parties in general) should create an organization whose sole purpose is to identify, gather, certify and disseminate such force-field parameters. This organization would 'belong' to no one, but would be of, by and for the scientific community as a whole. The idea is certainly attractive, however many pitfalls there might be in implementing it.

It is unrealistic in the extreme to assume that a single existing group could carry out such a project successfully. Too many tasks are involved. Its ultimate success would require the involvement of the entire scientific community. We have — here and now — the opportunity to enhance the practice of chemistry and (we can only hope) the condition of man. In short, we have the opportunity to help to forge the future.

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