WHAT IS RESEARCH?

The foundations of what we all understand as science are empirical. Stated simplistically: We measure things. Our scientific knowledge is derived from careful observation and measurement. Science is deeply rooted in this tradition.

We must, however, admit that the process of acquiring the knowledge on which society can move forward must be of a more complex nature. We can recognize a process by which all of our careful observations are related — and related in such a way as permits us to derive a far greater understanding of the physical universe than any observation, viewed singly, could ever provide. By this, I mean the process of synthesizing a theory into which we can fit our observations. The advantage of this process, obviously, is that it permits one to make predictions regarding hitherto unobserved phenomena. We can then conduct additional experiments for verification. Thus our knowledge pulls itself up by its own bootstraps.

Chemistry has a generalizing theoretical foundation, i.e., Quantum Mechanics, from which it can carry out this process. In principle, it should someday be possible to explain the vast body of observations which we know as chemistry on the basis of Quantum Mechanics. This statement does not imply that we will ever cease measuring things. We may simply make fewer measurements. We may measure different things — but we will still measure!

As our ability to make accurate calculations and obtain useful information about chemical entities increases, there will inevitably come a moment at which one group of chemists will question the significance of a physical reality obtained by another group of chemists working from a theoretical base. Consider the following scenario:

Two molecules wiht very similar structural characteristics are noticed experimentally to be very different with regard to their individual reactivities. One molecule is roughly a thousand times more reactive than the other, for reasons which are not clear. A situation of this type lends itself well to the use of computational methods. Just such a situation was recently confronted by a young researcher. Recognizing an opportunity to gain quick insight into the matter, the researcher carried out a series of MOPAC calculations which provided a fairly comprehensive explanation of the observed phenomenon. He then presented these results to his research director, whose attitude implied that the procedure followed didn't really count as research. The director insisted that the molecules in question be synthesized and their behavior analyzed using some established analytical technique. This was subsequently done — and the experimental results confirmed the computational results.

This brings one clearly to the question of what constitutes research. Is one doing research only if information is obtained by some 'accepted' (experimental) process? Can research not be done by obtaining chemical information from a computational viewpoint followed, if necessary, by experimental verification in certain key points? Can one not view computational tools as being at least on a par with NMR or Mass Spectroscopy?

The answers to the final two questions should clearly be in the affirmative. Computational Chemistry can provide a researcher with insights at a level far more fundamental than most experimental techniques. Unquestionably, computational tools can be misused to produce ridiculous results;

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however, the same may be said of complex analytical devices which nevertheless are accepted in the everyday practice of chemistry.

Perhaps what we now confront is nothing more than the need to develop the level of familiarity of the practicing chemist with the tools and opportunities provided by Computational Chemistry. It is also possible that these techniques differ so radically from those accepted by the current chemistry community that their acceptance will be hard won over a matter of decades. In either case, it will become necessary that the scientific community acknowledges that obtaining new information — by whatever means — is research.

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