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EDITORIAL 6

It is a great privilege, for me as Editor, to publish a paper by Professor Ted Benfey based on his keynote address to our society meeting in Columbia, South Carolina, last year. Ted Benfey, simply put, has been doing history and philosophy of chemistry since before most of us were born. I would happily give a biographical sketch of Benfey's career were it not for the fact that he does so himself in the course of his article.

In the space of a few pages he sweeps majestically through a discussion of determinism and indeterminism, and attempts to reduce chemistry to quantum mechanics, while drawing on diverse thinkers from Ernst Cassirer to Isaiah Berlin. Benfey considers molecular kinetic theory and the development of organic chemistry, tracing analogies between their respective historical developments. His essay moves through the ideas of change which, as he points out, is an essential aspect of chemistry, and which was viewed differently by the ancient Greek and Chinese philosophers.

Benfey concludes by providing a rallying all for the new discipline of philosophy of chemistry, namely that chemistry focuses on the establishment of order, the formation of bonds and all manner of complicated structures. Of course all these tendencies are only temporarily successful in the face of the second law of thermodynamics, but they are nevertheless supremely important for any particular molecule, crystal or indeed any living organism or society concerned.

Science ethics is an area of study which has come increasingly to the fore, partly out of sheer necessity, given recent developments in areas like genetic engineering. Many academic departments now offer courses in science and ethics, but just as chemistry has been largely ignored in the study of philosophy of science so it tends to be ignored in discussions on ethics. In the second article in this issue

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Jeffrey Kovac, a physical chemist, begins to explore what he calls the philosophy of chemistry as a profession. He claims that such a study is an essential prelude to any attempt to understand ethics in chemistry more deeply, given that many of the ethical issues faced are intimately connected with the way that chemists are defined as 'professional'. The case of the chemistry is particularly interesting because, as Kovac explains, chemists must "think with their hands" since their field of expertise generally remains connected to practical aspects. The wide scope of application of chemistry has meant that issues involving the professionalization of this science have a more established history as compared with physics and biology for example.

Kovac mentions the work of Shapin, who has explored science in the age of gentlemanly research when institutions such as the Royal Society were beginning to develop. These scientists could afford to be completely honest about their findings, whereas things are rather different in present times. As I see it, today chemists write articles partly with a view to future grant applications. It is not uncommon for an attempt to develop a new theoretical approach, for example, to result in failure while still not preventing the authors from cheerfully concluding that their results are "very encouraging". I am sure that Kovac's article will deepen and widen the discussion of ethics as it applies to the chemical profession.[1]

The following article by Bruce King explores a theme on which some work already exists in philosophy of science, although probably not enough (Humphreys, 1992, 1993, 1995). This is the notion that the classical dichotomy between experimental and theoretical work in science is being seriously eroded by the rapid growth and application of computational methods. Here it is as if one performs a form of 'empirical mathematics', to borrow a phrase from philosopher of physics Michael Redhead. The computational approach is theoretical, since it relies on use of the computer rather than physical experiments, but the nature of the computations frequently involves some form of data fitting, iteration, or plain trial and error, so as to render them almost distasteful to those who prefer analytical solutions. Indeed, many of the issues which surface in philosophical discussions on quantum chemistry are connected with just this hybrid nature of computational chemistry and the extent to which

the techniques can be regarded as truly ab initio or semi-empirical (Needham, 1999; Scerri, 1999).

Returning to King's article, his own response to this general issue is to propose an experimental/theoretical/computational trichotomy. The adoption of this idea could mean that computational work might be viewed by philosophers of science as an equal partner to the traditional areas of experimentation and theory, rather than being interpreted merely in terms of the traditional dichotomy. King draws on his own experience in mathematical approaches to chemistry, while examining developments in the area of borane chemistry and the generalized concept of aromaticity to which he has made significant contributions.

But he also stresses the difference between computational chemistry and mathematical chemistry and shows how he and his colleagues have succeeded in giving explanations of chemical phenomena in an area where computational chemistry alone has failed to provide such answers. The field of mathematical chemistry, as distinct from computational chemistry, is a relatively recent one in which King has been one of the prime movers. Interestingly, the University of Georgia at Athens is a world center for both approaches given the presence of King himself, and Dennis Rouvray in mathematical chemistry, and Fritz Schaeffer and his colleagues in computational chemistry.

In the 1960s a number of passionate debates erupted in the study of biological taxonomy, so much so, that Stephen Jay Gould was later moved to characterize the field as "names and nastiness" (Gould, as quoted in Dawkins, 1986, p. 275). To simplify matters enormously, phylogenetic classification seeks to identify essential genetic attributes of an organism and to base classification on such traits. Numerical taxonomy, on the other hand, attempts to classify on the basis of phenetic resemblances and on the basis of a weighted average of numerous such attributes without including phylogenetic ones. Both systems inevitably possess non-objective aspects. In the case of phylogenetic classifications, which are generally arrived at from the examination of amino acid sequences, the final outcome depends on the particular protein which is chosen to experiment upon.[2] In numerical taxonomy the choice of the various properties to

be examined and the manner in which the weighted average between them is computed invariably influence the final outcome.

The author of the final article in the present issue is the distinguished biologist Peter Sneath, a leading numerical taxonomist who participated in some of those earlier debates. Today Sneath continues to pioneer the use of numerical approaches to classification and in the present article he turns his approach towards the periodic table of the elements. His aim is to examine the virtues of a classification which avoids emphasis on one single criterion (atomic number) by analogy to the numerical approach in biology, which avoids any allegedly essential genetic features.

Sneath alludes to myself and others who have argued that one cannot deductively predict the periodic table from the core theoretical principles of this area of science, namely quantum mechanics.[3]

It is of some interest therefore to see whether a method of classification which eschews all mention of atomic weights, atomic numbers, or electronic configurations of atoms, can recover something of the periodic classification which is usually held to be obtained only through such a reductionist approach. Sneath seeks a numerical average involving a great number of the chemical and physical properties of the elements while deliberately omitting properties such as their atomic weights. He does not appear to be proposing an alternative approach to the classification of the elements but a complementary one which might provide answers to specific questions which the current table cannot provide.

If Sneath's findings presented here are correct, we learn that it is indeed possible to recapture much of the grouping of elements which we know from the conventional periodic table classification. Incidentally, it is rather gratifying to see an article which appears to be free of the 'hype factor', mentioned earlier in this Editorial, and to encounter an author who is more than willing to expose the possible failings and weaknesses of his approach and to share these features openly with the reader.

NOTES

1. A related area which Kovac does not actually touch on in his article but which I have begun to explore in my own work is that of 'science hype' as recently witnessed in the misleading announcements that atomic orbitals had been directly observed (Bard, 1999; Scerri, 2000).
2. This kind of possibility was amply demonstrated as recently as 1990 when Carl Woese and co-workers arrived at a fundamentally revised classification of all living organisms on the basis of examining one particular nucleotide sequence (Woese, 1990). This scheme appears to have gained some acceptance, although not surprisingly it is disputed by some biologists.
3. Bohr did not deduce electronic configurations from quantum theory and, regardless of what many contemporary quantum chemists claim, even today's route to electronic configurations, based as it is on the radically different quantum mechanics, still cannot strictly predict electronic configurations of specific atoms. At least it is not possible without the use of the aufbau principle to select basis sets that are likely to be useful or by recourse to previous knowledge of the kinds of basis sets likely to yield good results.

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