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THE NEW PHILOSOPHY OF CHEMISTRY AND ITS RELEVANCE TO CHEMICAL EDUCATION

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ABSTRACT: This article tries to analyze briefly the reasons why philosophy of chemistry has only recently emerged, whereas the philosophical study of physics and biology are far better established fields of knowledge. Some key issues in contemporary philosophy of chemistry are reviewed and the ways in which this new branch of philosophy of science can be of potential benefit to chemical education are discussed. [*Chem. Educ. Res. Pract. Eur.*: 2001, *2*, 165-170]

KEY WORDS: philosophy of chemistry; chemical education; reduction of chemistry; quantum chemistry; scientific explanation

INTRODUCTION

Since the start of the 1990s a new branch of philosophy of science has begun to flourish. (Scerri, McIntyre, 1997; Bhushan, Rosenfeld, 2000; Van Brakel, 2000). This is the philosophy of chemistry, a field which was at the forefront of scientific research before the turn of the twentieth century but which seems to have been largely eclipsed as chemistry came increasingly under the reductive spell of theoretical physics and quantum mechanics. In this short article I want to try to place the recent growth of philosophy of chemistry in the context of the growth of the broader field of philosophy of science and I want to begin to ask what benefits this new field might have for chemical education.

PHILOSOPHY OF SCIENCE

Many universities now have departments or perhaps sub-departments of philosophy of science. If not then philosophy departments will almost invariably have one or two faculty members who teach and do research in philosophy of science. Some of the central questions traditionally addressed in philosophy of science are whether science makes progress, how science differs from other fields of endeavor and the manner in which successor theories depose their predecessors. These questions have usually been approached in terms of what is viewed as the paradigm science, that is to say physics. In the past this endeavor went hand-in-hand with the emphasis on the syntactic, logical and axiomatic analysis of theories as recommended by the Logical Positivists, who were largely responsible for the professionalization of philosophy of science.

However, beginning with Popper, Kuhn, Feyerabend, Lakatos and other more recent philosophers, the Logical Positivist program has been abandoned and with it the emphasis on logical analysis and attempts at reconstruction of science from first principles (Popper, 1965, Kuhn, 1970, Lakatos, 1970). Whereas this gradual erosion of Logical Positivist ambitions has been occurring since the 1950's and 60's, the emphasis on philosophy of physics continues to prevail, although admittedly in a less evident form.

Of course philosophers of science have now become aware of the bias towards physics and there has been a growing attention to the philosophy of biology (Sober, 1993). But in their efforts to get away from physics, philosophers appear to have completely by-passed chemistry. Until very recently there has been very little interest in philosophy of chemistry and the implication seems to have been that there were no interesting methodological lessons to be learned from chemical science.

It is interesting to try to analyze why this situation should have occurred. One important factor, for which I believe that chemical educators and chemists themselves are partly responsible, is the mistaken view that chemistry has been reduced to physics, or more specifically, to quantum mechanics. Or rather, chemists like to have it both ways. They look up to quantum mechanics because it appears to grant legitimization from a more formal branch of science but are also quick to react when it is suggested that chemistry risks becoming extinct as a result of computational quantum chemistry.

But there are many reasons why philosophers ought to be interested in chemistry since in exploring questions such as whether biology or consciousness reduces to physics one cannot ignore the more immediate question of whether chemistry reduces to physics. If reduction even fails at the first hurdle, then there is little hope of achieving a more ambitious reduction like that of biology to physics.

In the past the reduction of one science to another one was examined, in philosophy of science, by asking whether the axiomatized laws of, say chemistry, could be strictly derived from those of the reducing science, physics (Nagel, 1961). However nobody has ever succeeded in axiomatizing the laws of these two sciences, let alone showing that the necessary derivation between the two formalized sets of laws exists. It is not even very clear whether chemistry has any laws to speak of apart from a few such as maybe the Periodic Law (Scerri, 1997a, 1998a). These failures have not deterred philosophers from assuming until quite recently that chemistry does indeed reduce to physics.

But actually the periodic law contrary to popular textbook presentations cannot be fully reduced to quantum mechanics. Although quantum mechanics and the Pauli Exclusion Principle can be used to explain the number of electrons which each shell around the atomic nucleus can accommodate, it has not yet been possible to predict the precise order of electron shell filling from first principles (Scerri, 1997 b). The fact that the 4s orbital begins to fill before 3d is an empirical fact, observed in spectroscopic experiments, which can be accommodated into the theory but not strictly derived (Scerri, 1994; Melrose & Scerri, 1996).

In addition, the move away from positivism in philosophy has opened the path for a more naturalistic form of philosophy of science which examines what scientists themselves might mean by attempts at reduction. To chemists and physicists the attempt to reduce chemistry is to be found in quantum chemistry, which began to develop with the work of Heitler and London immediately following the birth of quantum mechanics. With the advent of high powered computation there has been an increasing reliability in the predictions made in this field. Any up-to-date examination of the reduction or otherwise of chemistry must therefore examine the methodology, successes and limitations of ab initio quantum chemistry.

Still on the issue of reduction, the question of whether biology reduces to chemistry is one which is increasingly being answered affirmatively due to the success of molecular biology in accounting for the nature and mechanisms of heredity. But even within this rather limited part of biology serious problems remain to be solved if we are to say that reduction has been successful. It seems as if we now comprehend the chemical basis for the transcription and translation of DNA. The fact remains that in carrying out these processes DNA molecules must use a host of proteins which are themselves generated by the DNA. Where do the first proteins come from to allow the cycle to begin? Although some steps have been taken towards answering this and similar questions, the reduction of biology to chemistry is clearly in need of reassessment (Rosenberg, 1994).

Similarly, the study of what constitutes a scientific explanation, a topic to which I will return below, also benefits from considering the nature of typically chemical explanations. For example, there is the prevalent use of electronic configurations of atoms to give chemical explanations. Are these types of explanations autonomous to chemistry or do they possess any strict foundation in quantum mechanics as is commonly believed? Such a foundation may have existed when the Pauli Principle could be stated by saying that no two electrons in an atom or molecule could share the same four quantum numbers. But soon afterwards the Pauli Principle was generalized to state that the wavefunction for a system of fermions is anti-symmetric upon the inter-change of any two electrons. The older version of the Pauli Principle became strictly invalid, since individual electrons cannot be assigned four quantum numbers each. Only the atom or molecule as a whole possesses stationary states and to ignore this development is to commit the 'orbital fallacy', although this remains an extremely useful approximation at the heart of much computational quantum chemistry. But as a matter of principle atomic orbitals can no longer be said to physically 'exist' in anything except one-electron systems. Many-electron orbitals are ontologically redundant (Scerri, 1991). The fact remains however that orbitals and configurations are here to stay in chemistry at all levels. This conflict between the foundational status of orbitals and their continued use in chemistry is largely a philosophical question which has begun to be addressed in some recent studies. For example some authors have considered whether quantum chemistry and the orbital approximation supports a realistic or anti-realistic view of theoretical terms (Scerri, 2000b)

One can also look into the nature of typically chemical laws, if indeed such entities exist, in order to help address the question "what are scientific laws?". Does the Periodic law count as a scientific law in the same sense as Newton's laws of motion? Clearly the 'repetition' of elements embodied in the Periodic law is by no means an exact relationship and yet the Periodic Law provided Mendeleev with some of the most dramatic predictions in the history of science.

Mention of the Periodic law also brings to mind a long-standing controversy in history and philosophy of science, over the relative virtue of predictions and accommodations by scientific theories (Brush, 1998). Although it is popularly believed that scientific theories are given more credit for making successful predictions of hitherto unknown facts, rather than for accommodating already known data, this is challenged by many philosophers who claim that both prediction and accommodation should count equally in the acceptance of a new theory. For example, when the Davy Medal was awarded to Mendeleev by the Royal Society, the citation made absolutely no mention of Mendeleev's dramatic predictions of the elements gallium, germanium and scandium. In addition the medal was jointly awarded to Mendeleev and his rival Lothar Meyer, the latter of whom is known not to have made predictions of any new elements (Scerri, McIntyre, 1997). The formerly perceived immiscibility of chemistry and philosophy is now being challenged on a number of fronts as a result of developments both in chemistry and philosophy. It is time for philosophers and chemists realize that philosophy of chemistry has a great deal to offer. In fact there are now signs that this realization is beginning to dawn, as seen in the number of recent international conferences devoted to philosophy of chemistry. In addition two new international journals

Foundations of Chemistry and *Hyle* have now been established to cater for the new field as has the internet discussion list called '*philchem*'.

POSSIBLE BENEFITS TO CHEMICAL EDUCATION

The new developments in philosophy of chemistry are beginning to have an impact on chemical educators (Erduran, 2000a, 2000b). The reason why this should be so is rather obvious. If teachers want to teach chemistry more effectively the most productive approach for them to adopt, is to try to develop a deeper understanding of the subject matter that they claim to instruct others about. For example, and a chemical educator may be thought of as a person who provides scientific explanations and in particular chemical explanations. Most chemical educators have an intuitive feel for what an explanation means but would be hard put to try to analyze the concept of scientific explanation if they were asked specifically to do so. Meanwhile scientific explanation has been a major theme of research among philosophers of science, as mentioned earlier. The knowledge which has been gathered in philosophy of science would be of enormous benefit to chemical educators. The development of a form of philosophical self-examination of what goes into scientific explanations cannot but help educators to provide better explanations in the course of their teaching or perhaps provide a number of alternative explanations to reach different student audiences. In addition there is now work being conducted in trying to understand the peculiarities of chemical explanations and whether they follow the same general pattern as explanations in physics for example. Chemical educators will gain a great deal from familiarizing themselves with such research since it will enable them to be clearer in the way in which they present various aspects of chemistry to their students and colleagues. It is not enough to train chemistry teachers about just the contents of chemistry courses and perhaps a little educational psychology. Chemical educators need to be introduced to the study of the nature of chemistry.

PHILOSOPHERS' ACCOUNTS OF SCIENTFIC EXPLANATION

I would like to briefly mention the key views which have been described concerning the nature of scientific explanations. Perhaps the oldest established ideas on explanations in the sciences are those described as the covering-law model of explanation (Nagel, 1961). This account holds that a scientific explanation of any particular fact involves showing that it flows deductively from a certain known law of nature. As such this approach is in keeping with a formal logical approach of wanting explanations to be logically deduced from a set of premises, in this case a law or several laws of nature.

An alternative account which has received a good deal of attention has been the view that scientific explanations seek to provide unification (Kitcher, 1981; Friedman, 1974). There is of course a good deal of evidence for this view, especially from the field of physics where unification has been actively courted from the time when Maxwell showed that electromagnetism and light were just aspects of one underlying reality, namely the electromagnetic force. This program was of course extended by Einstein who sought, unsuccessfully as it happens, to unify the force of electromagnetism and gravitation. Today unification remains the holy grail of theoretical physics where the aim is to combine together not just the two forces which Einstein tried to join but also the strong and weak nuclear forces. When we turn to chemistry it is not quite so obvious that unification is always the hallmark of a successful chemical explanation. Chemistry by its very nature involves giving more specific explanations for a great diversity of reactions and types of substances. One is possibly not quite so concerned about unification in a field which is characterized by its very diversity. Of course one can have diversity as well as unification simultaneously as one observes very strikingly in the case of the periodic system of the elements.

A third approach to scientific explanations taken by philosophers of science has been a contextual view of scientific explanation. This view championed especially by van Fraassen recognizes that different explanations are given in different settings (van Fraassen, 1980). This would seem to be especially true in chemistry where rather than always seeking a fundamental explanation one is more often seeking a level specific explanation which speaks in a chemical language rather than in abstract terms of theoretical physics.

The more a chemical educator knows about the various dimensions of scientific, and in particular chemical, explanations the more effectively he or she can teach chemistry. Without any input from philosophy of science, the views of explanations which chemical educators possess must remain tentative, intuitive and largely ill-formed. By self consciously addressing the question of scientific explanation and drawing of the work which philosophers have carried out on this and similar topics chemical educator cannot fail to become more enriched in their broad understanding of chemistry. This is one of the many reasons why the new philosophy of chemistry is of great relevance to chemical education at all levels. It is because it introduces an element of close self-scrutiny and analysis which has been lacking up to the present time. Rather than merely introducing chemical educators to the nature of science in general, as has been advocated in many studies, they should be introduced, first and foremost, to the nature of their own science: chemistry. While it is essential for chemical educators to be familiar with the details of the many chemical theories, models and laws which they hope to teach, it is almost more important that they become aware of what theories, models and laws are in general and how they vary in nature among the basic sciences of physics, chemistry and biology. This is particularly important in view of the interdependence of the three basic sciences which nevertheless retain certain unique characteristics. Unless one is aware of these kinds of issues one might judge chemical theories in the same way as theories of physics and introduce serious misconceptions in the process of doing so.

Although many educators have advocated instruction in the Nature of Science for science educators this initiative has not been widely embraced (Duschl, 1994; Hodson, 1988; McComas, 1998; Matthews, 1994). Perhaps the advent of the new philosophy of chemistry, which is of more immediate relevance to chemical educators, will lead to renewed interest in a deeper examination of key issues and concepts of chemistry which are not directly concerned with pure chemical content. Rather than be exposed to philosophy of science which so frequently draws examples from physics and biology, chemical educators can now begin to appreciate the philosophy of their own science. The philosophy of chemistry has emerged after a long delay and many resources have now been produced which are waiting to be taken up and used by chemical educators (Scerri, 1997a).

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