CHAPTER 6

NORMATIVE AND DESCRIPTIVE PHILOSOPHY OF SCIENCE AND THE ROLE OF CHEMISTRY

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INTRODUCTION

Since the demise of Logical Positivism the purely normative approach to philosophy of science has been increasingly challenged. Many philosophers of science now consider themselves as naturalists and it becomes a matter of which particular variety they are willing to support. As is well known, one of the central issues in the debate over naturalism concerns whether philosophy offers a privileged standpoint from which to study the nature of science, or whether science is best studied by studying science itself.[1]

The situation is often summarized by the aphorism that one cannot derive an "ought from an is." It does not appear as though we should be entitled to draw normative conclusions about how science should ideally be conducted by merely observing the manner in which it is conducted at present, or was conducted in the past, since this appears to be a circular argument. Indeed the only circumstance in which the die-hard normative epistemologist would contemplate any input from naturalism would be if it could be shown conclusively that rational agents were literally incapable of thinking in the manner which the normative scheme requires that they should.[2]

I am speaking as though the normative approach is somehow more respectable and that naturalism represents a recent intruder onto the philosophical scene. I am suggesting that the burden of proof lies with the naturalists to show that their position can have some influence on normative philosophy and not vice versa. This may indeed be the case at the present time but things were not always this way. Normative philosophy and philosophy of science did not always hold center stage. It arose as a result of the work of Gottlob Frege in Jena at the end of the 19th century. Frege's development of modern logic rapidly led to attempts to base all of philosophy on the analysis of language, a program that was furthered by Russell, Wittgenstein, Carnap, and many others. Frege's program led to the overthrow of the then current naturalistic philosophy, which looked to scientific discoveries and scientific practice for philosophical enlightenment.

Before Frege, the study of psychology and evolutionary biology *were* indeed highly regarded among philosophers of the day. In particular, psychologism was not

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considered to be the 'mortal sin' that Frege later convinced analytical philosophers that it might be.

Today confidence in the analysis of the logical structure of scientific theories and the approach involving an *a priori* or a "first philosophy" has waned. Philosophers *do* now explore ideas from psychology, biology, physics, political science, economics, computation, and as it would appear are even beginning to consider the field of chemistry (van Brakel 2000; Bhushan and Rosenfeld 2000). These excursions may all be said to fall under the generic label of naturalism. The proponents of these approaches share an opposition to the Frege–Wittgenstein line whereby philosophy is somehow more fundamental than all these other branches of learning.

I want to spend a few more moments in exploring how the stranglehold that Frege had around analytical philosophy has been loosened. Frege's position may be stated in simple terms as requiring that:

(i) Logic and not psychology is the proper medium for philosophy.
(ii) Philosophical reflection is to be regarded as *a priori*.

Modern naturalists, not surprisingly, dispute both (i) and (ii). One of the main reasons why (i) has been reconsidered, and why there has been a return to psychologism, has come from work in epistemology. In 1963, Edmund Gettier presented some examples to show that there are cases when one might possess true and justified belief and yet fail to have knowledge (Gettier 1963). Philosophers like Dretske and Goldman have led the way in formulating responses to these puzzles that invoke the psychological states of knowing agents (Dretske 1981; Goldman 1992).

Meanwhile (ii) has been challenged on various fronts. First of all, Quine produced his famous articles in which he argued that the distinction between analytic and synthetic statements could not be clearly drawn (Quine 1951). As a result, any hopes of a completely *a priori* approach to philosophy would appear to be discredited. And yet in spite of other well-known contributions from Quine such as his slogan that "philosophy of science is philosophy enough," and his general support for a naturalized epistemology, his own work remained steeped in logical analysis and did not shown much sign of engaging in an examination of actual science.

Then came the historical turn in philosophy of science due to Kuhn, Lakatos, Toulmin, Feyerabend, and Laudan among others. These authors have done much to show the importance of the history of science to the study of scientific methodology. In addition, for better or for worse, the writings of Kuhn, in particular, have spawned the sociology of science and science studies industries which claim to study science as it is actually practiced and stress the need to go beyond an analysis of theories. I say for better or for worse because, as I see it, the problem with sociology of science has been an obsession with the context of scientific developments and the demotion of the actual science involved.[3] What many of these authors have done is to take naturalism a little too far such that they end up with relativism. This is of course one of the well-known dangers of naturalism in general.

Two leading current proponents of naturalism include Ronald Giere and Larry Laudan (Giere 1985, 1989; Laudan 1987, 1990). Perhaps, the main distinction between them seems to be that Laudan insists that his brand of naturalism is also normative whereas the claim to normativity is rather weaker in Giere's version, although not altogether absent as some commentators seem to believe.

Another author to champion naturalism has been Philip Kitcher. His 1992 article in the centenary issue of *Philosophical Reviews* presents one of the clearest accounts of the history of naturalism and the various currently available positions (Kitcher 1992). Kitcher followed this with a book called *The Advancement of Science* in which he claimed to be doing naturalistic philosophy of a moderate kind. But as some critics have suggested Kitcher seemingly fails to deliver the goods (Solomon 1995). The book is full of formal analysis of scientific episodes such as the Chemical Revolution and one cannot help wondering, as in the case of Quine's writings, where the real science might be lurking.

Of course there are still many philosophers, including Siegel and Doppelt for example, who continue to dispute the very notion of a naturalized philosophy of science (Siegel 1985, 1989; Doppelt 1990).

CHEMISTRY?

So much by way of introduction but what is the relevance of chemistry to these issues? First of all, if by naturalism one means looking at science itself, rather than purely operating within a logical analysis of concepts, then here in chemistry is a whole field of science that has never been seriously considered. The apparent disdain for chemistry is all the more surprising when one considers that chemists are by far the largest group of scientists among people studying and working in any of the sciences.[4]

But the main point I want to make in this article is that in a sense one *can* indeed derive "an ought from an is," although I intend this claim in a more restricted sense than usual. I will argue that by starting with a naturalistic approach to the nature of chemistry, we can make normative recommendations to chemists and chemical educators. The larger question of whether one may make normative claims about science in general is a more difficult one, which I will avoid for the time being. But if what I say about chemistry is correct then perhaps it could easily be generalized to other branches of science (Siegel 1985, 1989, 1990; Doppelt 1990).

FROM NORMATIVE TO NATURALISTIC

I have begun to realize that my own research in philosophy of chemistry has consisted in a gradual shift from initially advocating a normative view about such issues as atomic orbitals and electronic configurations, to more recently adopting a naturalized position. I now find myself advocating the critical use of such concepts rather than highlighting the fact that they strictly fail to refer to any entities in the physical world. Please allow me to now re-trace some of these steps in my own research.

In the case of a many-electron atom or molecule the commutator involving the Hamiltonian operator and the operator corresponding to the angular momentum of an individual electron, $[H, \ell_x]$, is non-zero. This implies that eigenvalues corresponding to the angular momentum operator for any individual electron is not a constant of the motion, or to use the jargon, is not a good quantum number, and cannot be said to characterize the motion with any exactness. For example, in the absence of spin–orbit coupling only the vectorial sum of all the individual angular momentum operators or L, rather than individual angular momenta, or ℓ, represent good quantum numbers. Another way of stating this result is to say that the individual electrons in a many-electron atom are not in stationary states but that only the atom a whole possesses stationary states. Similar arguments can be made for other quantum numbers like m_ℓ and m_s and these likewise imply the strict breakdown of the notion of assigning four quantum numbers to each electron in many-electron systems.

But more important than the approximate nature of the orbital concept is the categorical fact that an orbital does not refer to any physical entity. Here we are fortunate in having a clear-cut case where it is not left to one's philosophical prejudices as to whether we should adopt a realistic or anti-realistic interpretation. The mathematical analysis dictates quite categorically that the much beloved, and much pictured, concept of atomic orbitals does not have a "real" or independent physical existence. Indeed the use of the term "orbital" rather than orbit does not really convey the radical break with the notion of a continuous path for elementary particles, which took place as a result of the advent of quantum mechanics.

Of course it is still possible to use the complex mathematical expressions, corresponding to the different type of orbital solutions to the hydrogen atom problem, in order to build up a wavefunction that approximates that of a many-electron atom or molecule. In such cases, we are using orbitals in a purely instrumental fashion to model the wavefunction of the atom or molecule and there is no pretense, at least by experts in the field, that the constituent orbitals used in this modeling procedure possess any independent existence. Contrary to the recent claims which appeared in Nature magazine, as well as many other publications, orbitals have not been observed (Scerri 2000b, 2001).

Now what I have been arguing concerning orbitals, for several years, is a normative claim which emerges from paying strict attention to quantum mechanics. But soon after I started to publish these ideas, Robin Hendry, pointed out that according to some philosophical analyses of scientific theories my position was somewhat passé.

Hendry's criticism of my article of 1991 went something like this.[5] He claimed that the issue I was raising did not have quite the philosophical significance that I was attaching to it. Whereas I was pointing out that the realistic interpretation of one-electron orbitals was strictly inconsistent with quantum mechanics, Hendry claimed that in making this assessment I was working within the covering-law model of explanation. This model appeals to fundamental laws for explanation or, in the case I am considering, the Schrödinger equation. Hendry's view, following Nancy Cartwright, was that it is not fundamental theories or laws that explain but scientific models. Of course this represents another version of naturalism. Nancy Cartwright has championed the view that it is models, rather than scientific theories, that are used in scientific practice to give explanations for natural phenomena (Cartwright 1983).

To connect this with my main theme, I am saying that my own normative approach has been to claim that the fundamental theory explains everything. Hendry countered this claim by appealing to Cartwright-style naturalism which required that we look carefully at the way that models are used. As Cartwright correctly points out, it is often models that scientists appeal to rather than high-level theories. From the normative perspective based on the theory there is indeed something wrong with the way in which the orbital approximation is used in many areas of chemistry and even applied physics. But from the perspective of what I shall call Cartwright–Hendry naturalism, scientists regarding orbitals realistically cannot be faulted given the central role of models in modern science. I did not readily accept this criticism at the time when Hendry first circulated his manuscript but recent developments in my work have now shown me that he was making a very valuable point (Hendry 1994).

In addition, some chemical educators have reacted to my work by pointing out that orbitals are here to stay and that no amount of nit-picking about whether or not they exist physically will have the slightest impact on their use in teaching chemistry (Richman 1999a,b; Emerson 1999). Of course my thought had never been that we should do away with orbitals but that we should point out more carefully their limitations in the course of teaching chemistry.[6] From a philosophical point of view the aim was to examine objectively the theoretical status of electronic orbitals and configurations from the perspective of quantum mechanics.

Then one day some years ago while giving a lecture on philosophy of chemistry a thought came to me. The thought was that it is quite appropriate for chemists and chemical educators to not only use orbitals but to do so in a realistic fashion regardless of their status according to the fundamental theory of quantum mechanics. I think, I fully realized at this moment the truly paradoxical situation in that chemistry is an autonomous science while at the same time resting on fundamental physics. These two positions need not be seen as being contradictory just as the normative and the naturalized position need not be seen as contradictory.

In 1997, I met Bernadette Bensaude, the well-known French philosopher of science, whose work is motivated by the history of chemistry. We struck up a conversation about Paneth and his view of the elements which is the subject of one of the classic papers in philosophy of chemistry written in German and translated by his son Heinz Post (Paneth 1962)[7]. The gist of Paneth's paper is that the chemist must adopt an intermediate position between the fully reductive view afforded by quantum mechanics and a naively realistic view that dwells on colors, smells, and such-like properties of macroscopic chemistry. In that paper, Paneth is concerned with how elements are to be regarded and he upholds a dual view of elements as unobservable "basic substances" on one hand and observable "simple substances" on the other. This he claims resolves a major puzzle in the philosophical understanding of substance, namely how it is that an element can survive in its compounds although the properties of the compound appear to bear very little resemblance to those of the element.

I suggest that this is a way of seeing the relationship between a normative view, or what quantum mechanics says about chemistry, and the more naturalistic view which tries to consider how chemists and chemical educators actually regard chemical concepts and models. Although it may seem paradoxical to embrace both positions at once, perhaps one might rest easier with Paneth's view of an intermediate position. But my emphasis, contrary to Paneth's conciliatory stance, is that both positions should be adopted simultaneously. Admittedly the history of paradox has a long history in Western thought. Usually a paradox is regarded as a serious problem that must be struggled against and overcome at all costs. Interestingly in Eastern thought, especially Chinese philosophy, paradoxes are not serious dilemmas to be resolved. Instead a paradox is to be embraced for what it is. It is in this rather esoteric sense that I am proposing to regard the reduction of chemistry, on one hand, and the continued use of reduced concepts as being paradoxical.[8]

In the 1960s and 1970s, Kuhn and others showed philosophers of science that it was futile to insist on a normative view of scientific theories which did not bear much relationship to the historical development of real science. Similarly, the case of atomic orbitals, which I continue to concentrate upon, shows us that it is somewhat unhelpful to insist only on the normative view from quantum mechanics. One needs to also consider what is actually done in chemistry and the fact that chemists get by very well by thinking of orbitals are real objects. In fact we need both views, the normative and the descriptive. Without the normative recommendation orbitals are used a little too naively as in the case of many chemical educators who do so without the slightest idea that orbitals are strictly no more than mathematical fictions. Hopefully my previous work was not in vain if I have managed to convince some people in chemical education to be a little more careful about how far an explanation based on orbitals can be taken.

To make a general point now, I think it is still of great value to question the status of the orbital approximation even if one eventually returns to using it in a realistic manner in chemistry. This is because the eventual use of the orbital approximation is greatly improved by such questioning.[9]

FROM NATURALISTIC TO NORMATIVE: THE REDUCTION OF CHEMISTRY

There is another area in philosophy of chemistry where I have been urging a naturalistic approach ever since the beginning of my work. This concerns the question of the reduction of chemistry to physics or more specifically quantum mechanics or relativistic quantum mechanics if one insists on being very precise.

As far back as the 1994 PSA meeting in New Orleans I suggested that the reduction of chemistry should not be regarded in the classic fashion of trying to relate the theories of chemistry to the theories of physics or in the formal sense of seeking bridge principles (Scerri 1994). The problem with such a Nagelian approach is that it requires axiomatized versions of the theory to be reduced as well as the reducing theory. Now although a case can be made for the existence of axiomatic quantum mechanics, clearly the same cannot be said for chemistry since there is no axiomatic theory of chemistry.[10]

But my main reason for advocating a naturalistic approach was that scientists themselves have an entirely different approach to the question of whether chemistry has been reduced to physics. Instead of considering a formal approach linking the theories in both domains a scientist would try to examine the extent to which chemically important quantities such as bond angles, dipole moments and the like can be derived from first principles from the reducing theory or quantum mechanics. A more challenging question for the theory is whether the liquidity of water, for example, can be predicted from first principles. One suspects that this will remain unattainable for some time to come or even than it may never be achieved. Rather than seeking a relationship between theories, a naturalistic approach to the question of the reduction of chemistry should examine the relationship between chemical properties on one hand and the reducing theory on the other hand.

Of course the hope is to go beyond data such bond lengths or dipole moments and to be able to calculate the feasibility or rate of any particular reaction from first principles without even needing to conduct an experiment. It should be mentioned that considerable progress has been made in the quantum theoretical approach to reaction rates although very accurate treatments have, not surprisingly, been confined to such reactions as that of hydrogen atoms with hydrogen molecules.

Since making this proposal I have found many instances of philosophers who have hinted at precisely this more naturalistic, more pragmatic, approach to reduction which consists in following what computational chemists and physicists do (Suppes 1978; Popper 1982; Hacking 1996). To repeat, whereas philosophers have previously viewed reduction as a relationship between theories, the naturalistic approach I advocate consists in accepting the scientific approach to the reduction of one branch of science to another but without sacrificing any philosophical rigor in analyzing the procedures used. Indeed what begins as naturalism can, I claim, turn to making specific normative recommendations to practitioners in the fields such as computational quantum chemistry (Scerri 1992a, b; 1998a, b). What I discovered was that in many instances in computational quantum chemistry chemists were claiming strict deduction of chemical facts from the Schrödinger equation. But such treatments frequently involved semi-empirical procedures such as using a set of orbitals that are found to work in other calculations or the use of calculations that fail to estimate rigorous error bounds (Scerri 1997). I will not enter into further technicalities here. But I want to suggest is that this is an example of moving in the opposite direction. What begins as a naturalistic or descriptive project ends up by making normative suggestions.[11]

CONCLUSION

I am suggesting that both the normative view about the status or orbitals according to quantum mechanics, and the adoption of a realistic view of orbitals can happily coexist. This I claim is an example of the coexistence of the normative and naturalistic approaches to philosophy of science. This claim will only appear to be a contradiction if one maintains the usual static view about holding philosophical positions. There have recently been signs that philosophers have grown tired of the never-ending arguments regarding realism and anti-realism since they realize that both positions show many virtues. Arthur Fine has coined the phrase "Natural Ontological Attitude"

(Fine 1986). On my reading the important part of this notion resides in the choice of the word "attitude" rather than position and although Fine has not really developed a distinction between attitude and position his articles hint in this direction. What I believe Fine is getting at is that we should no longer think of the discussion as an either/or situation between realism and anti-realism but rather that scientists adopt both positions at different times and sometimes even both at once. These are not so much positions held by scientists and philosophers but the more temporary, more dynamic, attitudes.

I think that this suggests an even further stage in the kind of bootstrapping I have been urging in this paper. The nature of chemistry, more than physics or biology perhaps, could serve as a model for the kind of philosophical approach based on "attitudes" rather than hard and fast positions which one is typically supposed to maintain and defend at all costs. This seems especially appropriate since chemistry, as its practitioners, as well as chemical educators know only too well, requires us to operate on many different levels simultaneously. It demands the adoption of several attitudes. To show you what I have in mind let me end by quoting from the work of a South African chemical educator Michael Laing:

> The difficulty arises because we teach chemistry simultaneously on four different levels, The Realities of Water.
>
> Level 1: macroscopic: tactile (touchable, tasteable, wet to the touch).
>
> Level 2: communicative: language, name: (a) oral and aural, the word, the sound assigned to something that can be seen and felt; and (b) the written version.
>
> Level 3: symbolic, representational: elemental formulaic. This came once chemists understood the concepts of elements, atom, equivalence, valence, stoichiometry, beginning n 1800 and understood by 1860 as confirmed at the Karlsruhe conference. Wet water now becomes H_2O with a relative molecular mass of 18 units. Numeric calculations become important.
>
> Level 4: Atomic scale model. This representation depicts the shape and size of the molecule on a scale so small that it s beyond the comprehension of the average person . . . .
>
> To appreciate water as a chemist you must make use of all four conceptual levels and be able to switch from one to the other as appropriate (Laing 1999).

Chemistry is a fertile new area in which philosophy of science could investigate further the question of normative and naturalistic approaches or the question of whether or not scientists actually adopt philosophical positions in the manner in which they use and interpret scientific theories. My own feeling is that chemists, in particular, tend to adopt different "attitudes," to use Fine's phrase, depending on what level they are operating at.

NOTES

1. The term naturalism has a variety of meanings. For example, in the philosophy of the social sciences it is sometimes taken to mean positivism. This is not the sense in which naturalism is being used in the present article. I am not concerned here with an empirical approach to social science but with a form of naturalism that involves concentrating on the apparatus, techniques, and assumptions of the natural sciences.

2. I am grateful to Martin Curd or Purdue University for discussion on this point.
3. An analogous situation exists in chemical education research at present with nearly all efforts being directed toward the learning process and virtually none at the content of chemistry courses (Scerri 2003).
4. Even sociologists of science appear to have overlooked chemistry, with the possible exception of Bruno Latour's book laboratory life, which is based on observations made in a leading biochemical laboratory (Latour and Woolgar 1979).
5. The article in question is Scerri (1991).
6. In addition, contrary to what Hendry claimed in his article I did not advocate the use of more rigorous forms of quantum chemistry for chemistry at large.
7. See Ruthenberg's short biography of Paneth (Ruthenberg 1997).
8. Needless to say I am not an advocate of parallels between modern science and Eastern mysticism as popularized by the likes of Capra and Zukav (Capra 1976; Zukav 1979). For example see my critique of the alleged parallels between Eastern mysticism and modern physics as published in the American Journal of Physics (Scerri 1989).
9. A recent article by Lombardi and LaBarca analyzes my position on the status of atomic orbitals as well as building on my view (Lombardi and LaBarca 2005).
10. This has not prevented philosophers from trying to axiomatize certain parts of chemistry, such as the Periodic system of the elements for example (Hettema and Kuipers 1988). See also the following critique of these attempts (Scerri 1997).
11. Let me also mention that Paul Needham has produced a detailed critique of my view on the reduction of chemistry in a debate between us which has been published in several issues of the International Journal for the Philosophy of Science (Scerri 1998b; Needham 1999; Scerri 1999; Needham 2000; Scerri 2000a).

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