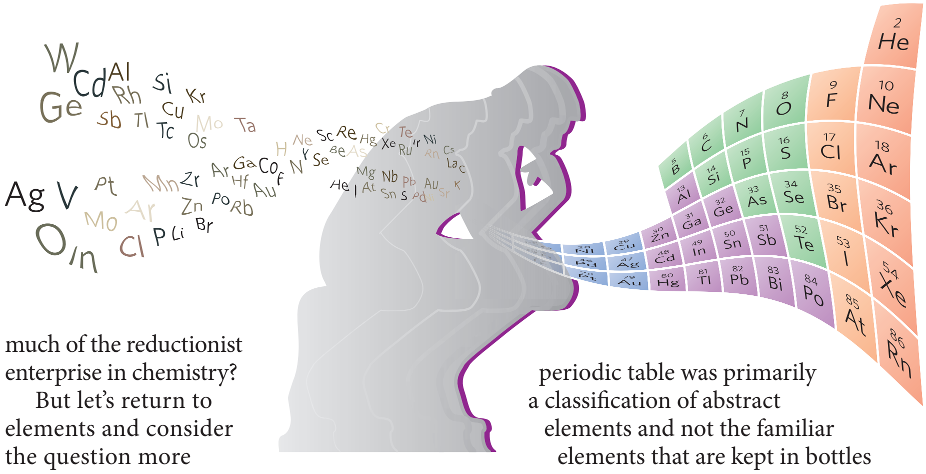
Chemistry goes abstract

Can philosophy make worthwhile contributions to science? **Eric Scerri** thinks it can, and looks at what it has brought to the table for chemistry.



Some years ago I bought a T-shirt at an American Chemical Society meeting that read, 'Philosophers Ponder and Chemists React'. Like so many jokes and aphorisms, this pretty much hits the nail on the head, although it can be read in many ways — one being that philosophers achieve nothing compared with chemists. As someone who is working in the burgeoning field of the philosophy of chemistry, I want to explore this idea a little further and ask about the relationship between philosophy and chemistry.

Chemists are often sceptical of philosophy, and rightly so when it comes to armchair philosophy or — to give it its more grandiose label — analytical philosophy. But in recent decades, some analytical philosophers have increasingly turned to science as a basis for their analyses and pronouncements.

This naturalistic turn can be variously attributed to Quine, Popper or Kuhn, three giants of twentieth-century philosophy each of whom stressed a different aspect of why philosophers need to look closely at the work done in science. Nevertheless, some contemporary scientists are still not impressed and are fond of declaring that philosophy has achieved nothing worthwhile. But are they correct? I believe not and I will briefly consider some issues in the philosophy of chemistry, the most recent of the philosophies of the special sciences[1,2].

Two central themes in chemistry are, of course, the chemical elements and the periodic table. In both cases, their significance both in chemical education and chemical research are usually taken for granted and unworthy of further thought. Let me start with the elements and a central question in the philosophy of chemistry. How is it that the poisonous element sodium combines with the poisonous non-metal of chlorine to form a compound that is essential for life? This seems to be a good candidate for 'emergence' in chemistry, namely the notion that the properties of the whole cannot be deduced from those of the parts. The response from some chemists is that it has all been explained by the modern theory of bonding and quantum mechanics. And yet to the best of my knowledge nobody has yet predicted the properties of NaCl, such as it being non-toxic, its colour, its taste and so on. Is this asking too much of the reductionist enterprise in chemistry?

But let's return to elements and consider the question more deeply. First it is necessary to begin with a clarification of the concept of 'chemical element', an issue that has been debated since the dawn of ancient Greek philosophy. Briefly put, elements have been regarded in at least two main ways. First they have been considered as abstract — some say metaphysical — principles that underlie the familiar observable elements. The other conception is one of elements as 'simple substances', that is to say, the tangible and observable elements that can be isolated and with which one is generally familiar, such as gold, oxygen, iron and so on.

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Perhaps one of the most important contributions made by Lavoisier during the chemical revolution was his placing a greater emphasis on the observable sense of 'element' and to downplay the rather mysterious abstract concept of the elements. Nevertheless, the more abstract concept was not fully abandoned and continued to have a fundamental role, especially in the hands of Mendeleev's later discovery of the periodic system. Mendeleev insisted that the periodic table was primarily a classification of abstract elements and not the familiar elements that are kept in bottles and flasks. For example, he argued that the place labelled as 'C' in the periodic table did not denote either diamond or graphite — the two then known allotropes of carbon — but instead carbon as the abstract element.

At the start of the twentieth century, isotopes of the elements were discovered. This initially posed a threat for the periodic table because the number of 'simplest' atoms seemed to be proliferating at a quick pace. Again it was realized that by concentrating on the abstract conception of 'element' rather than on individual isotopes, the validity of the periodic table remained unscathed. One of the leading contributors to the resolution of this question was the Austrian radiochemist Friederich Paneth, who also published a highly influential philosophical article that has been the starting point in many studies in contemporary philosophy of chemistry[3–5]. Paneth reminded his readers of the need for a dual conception of the term 'element'; he introduced new terminology into the discussion and distinguished the two senses as carefully as possible.

This crucial distinction is well known and appreciated in the French system of chemical education where the term 'element' is used exclusively to denote the abstract sense. Meanwhile the other sense of what we know as 'element' in the Anglophone world is consistently called *corps simple* or 'simple body'[6]. But this distinction is sadly lacking in the English-speaking world, to the detriment of students struggling to understand how one and the same 'element', or so they are led to believe, can exist in such a schizophrenic way. And nor is the IUPAC definition of an element any more enlightening on this question. Indeed, even Paneth's translator seems to confuse the issue by calling simple bodies 'elements as basic substances', as Joseph Earley has recently pointed out[7].

Let me now go back to the periodic table, that wonderful icon of chemistry that is so coveted by other scientists. Is there any sense in which one optimal form of the periodic table may exist, even in the face of the 1,000 or so versions that have been published and with many of them claiming superiority? Well it depends on one's philosophical view on elements and the periodic system. If one is a realist, as many scientists claim to be, then it is surely consistent to believe that the periodic table is a representative of an objective — albeit approximate — repetition in the properties of the elements as one moves through the sequence of increasing atomic numbers. If this is indeed so, then there may well be an optimal table to reflect periodicity as it really exists in nature, even though we may not yet have discovered it.

Perhaps the much-debated position of hydrogen in the periodic table (group 1 or 14 or 17) is not a matter of choice, but rather a matter of fact that has just not yet been definitively settled. In many cases chemists seem quite content to ignore such questions, some even claiming that the periodic table is a human construction made for our convenience and thus rendering it meaningless to ask for one objective 'best table'. If anything, it is the philosophers of chemistry who are more active over such issues, whereas the chemists sit back and ponder a little, but are seldom prepared to get excited about such questions.

Similarly, it may be that the precise membership of group 3 can be settled in favour of either Sc, Y, La, Ac (ref. 8) or what seems to be the better-supported alternative of Sc, Y, Lu, Lr (refs 9,10). Also, if helium correctly belongs in group 2 rather than group 18, then we can all embrace the wonderfully elegant left-step periodic table rather than leaving it as a curiosity for some physicists and group theorists who place greater emphasis on electronic structure and formal symmetry than on chemical properties.

This brings us back to the question of reduction. To what extent is chemistry nothing but quantum physics? Chemists are strangely ambivalent on this issue. They accept reductionism up to a point because of the undoubted advantages that theory and theory-based computation have brought to the field. But they instinctively recoil at the suggestion that chemistry is fully reduced — even in principle. This too is a philosophical issue and one with ramifications in the debates over how to teach chemistry and what constitutes good chemistry research.

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Let me end with another specific issue having to do with the periodic table. Chemistry textbooks create the impression that the periodic table is fully explained by quantum mechanics. It is claimed that whereas Mendeleev had to grapple with the grubby properties of the elements to arrive at the periodic table, these days it all falls out of quantum mechanics and the fact that successive electron shells can hold a maximum of 2, 8, 18 and 32 electrons, respectively. This in turn comes from the possible combinations of the three spatial quantum numbers as well as Pauli's fourth quantum number, subsequently associated with electron 'spin'.

What is not often conceded is that this cosy explanation goes only so far, and does not account for the fact that all period lengths repeat, except for the first short period of just two elements. To explain these facts requires the use of the Madelung or $n + \ell$ rule — and this has yet to be theoretically deduced. In fact the relevance of the Madelung rule has recently been brought into question by a prominent quantum chemist who has been taking an active interest in the work of philosophers of chemistry. Eugen Schwarz has first of all emphasized that the rule applies to just neutral gas-phase atoms and not to atoms as they occur in compounds[11]. More startlingly he has uncovered a fact that seems to have escaped nearly everybody else. Eugen Schwarz points to Moore's tables of atomic energy levels to show that contrary to the common textbook statements, the 4*s* orbital does not fill before the 3*d* orbital. Of course, he might have stumbled across this fact in any case, but seems to have been motivated by calls to examine the theoretical status of the Madelung rule by philosophers of chemistry.

The philosophy of chemistry does have its uses. It helps to clarify conceptual as well as terminological issues and it contributes substantially to making improvements in chemical education. Finally, it even contributes to chemical research. For example, it may allow us to arrive at an optimal periodic table that would serve to highlight chemical similarities that remain obscure while we continue to use periodic tables in which some elements are incorrectly placed[12,13]. ❐

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