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What is an element? What is the periodic table? And what does quantum mechanics contribute to the question?

Eric R. Scerri

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Abstract This article considers two important traditions concerning the chemical elements. The first is the meaning of the term "element" including the distinctions between element as basic substance, as simple substance and as combined simple substance. In addition to briefly tracing the historical development of these distinctions, I make comments on the recent attempts to clarify the fundamental notion of element as basic substance for which I believe the term "element" is best reserved. This discussion has focused on the writings of Fritz Paneth which are here analyzed from a new perspective. The other tradition concerns the reduction of chemistry to quantum mechanics and an understanding of chemical elements through their microscopic components such as protons, neutrons and electrons. I claim that the use of electronic configurations has still not yet settled the question of the placement of several elements and discuss an alternative criterion based on maximizing triads of elements. I also point out another possible limitation to the reductive approach, namely the failure, up to now, to obtain a derivation of the Madelung rule. Mention is made of some recent similarity studies which could be used to clarify the nature of 'elements'. Although it has been suggested that the notion of element as basic substance should be considered in terms of fundamental particles like protons and electrons, I resist this move and conclude that the quantum mechanical tradition has not had much impact on the question of what is an element which remains an essentially philosophical issue.

Keywords Element · Basic substance · Paneth · Quantum mechanics · Periodic table · Madelung rule

Let me start with the first question, what is an element? We think we all know what elements are. They are things like hydrogen, oxygen, mercury, gold and uranium from which all compounds and consequently all substances are made. They are the building blocks of the whole universe. Of course all this is true but I want to dig a little deeper. I

E. R. Scerri (✉)
Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA 90095, USA
e-mail: scerri@chem.ucla.edu

want to adopt the perspective of a philosopher who questions the seemingly obvious and see where it might lead.

The philosophers of chemistry and others who have thought about this question have arrived at a dual sense of the word ‘element’ and this is what I want to start discussing. Let me begin with the more obvious sense of element which I alluded to above, the simple building blocks of compounds like hydrogen, oxygen and gold. This sense of the term element is relatively new in the history of science. In earlier times an element took on a more abstract and metaphysical sense. Philosophers from the time of Empedocles proclaimed that there were four elements, namely air, water, fire and earth. They even identified these elements in a one-to-one relationship with each of the original four Platonic solids, the octahedron, the icosahedron, the tetrahedron and the cube, respectively. When a fifth Platonic solid, the dodecahedron, was discovered by the ancient Greek philosophers, they decided that there had to be a fifth element which they named the ether. The Greeks believed that all substances were made from these four and later five elements but not only in a compositional sense. They also believed that the four or five ‘elements’ mentioned were the metaphysical ‘substances’ which stood underneath all other substances, and which were the bearers of all kinds of properties.

Such views went though numerous modifications and continued to hold sway well into the Middle Ages and among the alchemists. Then the scientific revolution took place and ancient knowledge was rejected. Observation became the characteristic of modern science. Metaphysical notions were gradually banished to be replaced by theories based on what could be measured and what experiments indicated. In spite of some much disputed contributions from Robert Boyle (Chalmers 2010, 2011; Newman 2010), it appears that the radical break in the concept of what constitutes an element took place at the hands of Antoine Lavoisier during the chemical revolution. Lavoisier was among the first to clearly stipulate that an element should be regarded as the final stage of chemical decomposition. He exemplified this notion by showing that one of the classical elements, water, was in fact composed of two element, oxygen and hydrogen, which unlike water were not capable of further decomposition.

So much for one sense of the term element, the more obvious one that I mentioned at the outset. Let me return to the more subtle sense which survives to this day and does much useful work in science, although chemists tend to initially deny its very existence. The second notion is one of an element as an abstract entity, a bearer of properties, some still say of an essentially metaphysical character, that underlies the other more direct and more mundane sense of Lavoisier’s element. In fact the more abstract sense of element never went away although attention was diverted to Lavoisier’s more tangible sense for some time.

One chemist who insisted on retaining an abstract sense of the term ‘element’ was the discoverer of the periodic table, the Russian chemist Dimitri Mendeleev. Mendeleev repeatedly stressed the importance of thinking about elements in an abstract sense in his writings and indeed proclaimed, rather counter-intuitively, that this more fundamental sense of element is what the periodic table is primarily classifying.

In fact Mendeleev’s message is as relevant to modern chemistry as it was in the 1860s when he began to publish on the subject. But how can this be? Surely abstract notions of elements as bearers of properties, with no actual properties per se have no role to play in our modern world based uniquely on observations. Such a view is not only limited but can be shown to be inconsistent with the periodic table in a very simple way.

Consider first the fact that the modern periodic table is based on the principle of one element occupying one space. This being the case, there is no separate place in the periodic table for the various allotropes of an ‘element’ like carbon. All three currently recognized allotropes which are diamond, graphite and buckminsterfullerene, must all be accommodated into a single space. So what is the carbon that is indicated when one points to the symbol C occupying the sixth place in the periodic table? The simple answer is that it is none of these separate allotropes but in fact the abstract essence of carbon that underlies all three allotropes and perhaps even new as yet undiscovered allotropes.

Similarly one can consider the question of isotopes of an element. Let us remain with carbon. The three most abundant isotopes of this 'element' are ^{12}C, ^{13}C and ^{14}C. But again the periodic table is based on "one element one place" and so any contemporary chemist has to concede that when he or she points to the sixth place in the periodic system they are not pointing to any physically existing isotope but to an abstract entity which somehow embodies all the isotopes of carbon.

It has been suggested that Mendeleev's pre-eminence in the discovery of the periodic table and his successful prediction of many hitherto unknown elements was due to his more philosophical, more abstract understanding of what an element really was. Had he been more of a positivist and had he restricted himself to just the elements in the sense of Lavoisier, or the 'simple substances', Mendeleev might not have been so far-seeing and nor would he have dared to correct the atomic weights of numerous other elements (Scerri 2007).

Although Mendeleev's message was largely forgotten, it was kept alive by some more philosophically minded chemists, one of them being the 20th century radiochemist Fritz Paneth. Paneth authored an influential article on the concept of an element in German in the 1930s. It appeared some 30 years later in English translation in the *British Journal for the Philosophy of Science* and has served as the focal point for all subsequent research on this question during the current revival in the philosophy of chemistry starting in the early 1990s (Paneth 1962).

Here are a few quotations from the Paneth article,

> I consider it helpful to distinguish two senses in which the expression "chemical element" is used by the terms simple substance and basic substance (Paneth 1965, p. 65).

> I suggested that we should use the term "basic substance" whenever we want to designate that which is indestructible in compounds… and that we should speak of a "simple substance" when referring to the form in which such a basic substance, not combined with any other, is presented to our senses (Paneth 1965, p. 65).

> We cannot ascribe any particular qualities to an element as a basic substance, since it contributes to the production of an infinite variety of qualities which it exhibits both when alone and in combination with other basic substances… (Paneth 1965, p. 65).

> With the concept of simple substance we may remain within the realm of naive realism. When we are concerned with the basic substance, however, we cannot disregard its connection with the transcendental world without getting involved in contradictions (Paneth 1965, p. 66).

I do not have the time to justice to the contemporary literature based on Paneth's paper on this occasion but I will mention some broad lines. The first thing to note is that there continues to be much disagreement about terminology as well as substance if you will excuse the pun. Some authors are happy to support Paneth's view that elements as 'basic substances'[1] are of a metaphysical nature (Earley 2005; Scerri 2005; Ruthenberg 2009).

[1] This term is the English translation of Paneth's "Grundstoff" as suggested by his son Heinz Post.

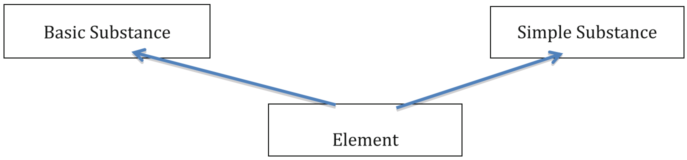

Fig. 1 Incorrect view, implied by some of Paneth's statements on the nature of 'element'

Others, working in the analytical tradition dispute the talk of metaphysics and prefer to say that this sense of the term element refers merely to a more abstract entity than simple substances (Hendry 2005, 2006; Vihallem 2011).

What I wish to do here is to suggest a possible criticism of Paneth's view and to connect this with contemporary work that is being carried out by some mathematical chemists who take a rather specific approach to the elements and the periodic table. Although the relationship between basic substance and simple substance has been much discussed, there is a certain amount of confusion between basic substance and 'combined simple substance'.[2] As I see it, some authors seem to conflate the two notions.

There are even some passages in the Paneth paper that contribute to this confusion. For example, Paneth writes,

> …I have preferred to speak of basic substance and simple substance as different aspects of the chemical concept of element (Paneth, p. 133).

This could be interpreted to mean that 'element' is the fundamental entity, while basic substance and simple substance are somehow derivative or maybe that basic substance is 'combined simple substance' both of which are incorrect (Fig. 1).

Moreover Paneth writes,

> Thus, in terms of the distinction introduced here, we may refer only to a natural system [periodic system] of basic substances not of simple substances. (Paneth 1962, p. 152)

I regard this statement as being too extreme. Basic substances underlie both combined simple substances and simple substances. The natural system (i.e. the periodic system) is as much about combined simple substances as it is about simple substances.[3] The properties of simple substances also show periodicity. e.g. group 1 metals. Their reactions with water, their physical properties, the fact that they show peaks in an atomic volume graph etc. Paneth's insistence that the periodic system only classifies elements as basic substances invites the obvious question of how we might learn about these elements, especially as they are said to have no properties. Admittedly atomic number provides an ordering criterion but periodic classification is also about group similarities which are recognized through the properties of elements as both simple substances and as combined simple substances. It is difficult to see how focusing primarily upon elements as 'basic substances' can provide any indication of the second dimension of the periodic table, namely the grouping of elements into vertical columns. An appeal to actual properties of the combined simple substances

[2] I am introducing this new terminology in the hope of achieving greater clarification.

[3] I thank a reviewer for encouraging me to think more carefully about this terminology. Whereas I have spoken of "combined element" in several lectures and the earlier draft of this paper, I now think that "combined simple substance" may be a more appropriate term. This means that the term 'element' could be reserved to only mean 'basic substance'.

and purely simple substances was the approach actually taken by Mendeleev and other pioneers of the periodic system.

Can we identify 'basic substances' with microstructural components of atom?[4]

It is certainly tempting to answer the above question in the affirmative. After all, the nature of basic substances may have been beyond observation in the early history of chemistry when only macroscopic properties could be observed. As later sections of this paper will argue, the quantum mechanical explanation for chemistry, and more specifically for the periodic table, is largely successful. It is reasonable to therefore suppose that modern chemistry and physics have succeeded in identifying basic substances and that they are the familiar proton, neutron and electron, the number of which distinguish the various elements and their isotopes?

Such an identification would enable one to interpret Paneth's writing on basic substances in a more concrete fashion and might avoid any apparent metaphysical excesses. However, I wish to resist making this identification, even at the risk of retaining some mystery. First of all, Paneth himself was well versed in the microstructure of atoms even if he may not have been a practicing quantum mechanician. Nevertheless, Paneth consciously resisted making any microscopic identification of basic substances along the lines suggested above. Quoting one H.C. Hell, Paneth writes,

> "According to the second definition…the concept of element coincides with that of atom, and serves mainly to designate and individualise the latter more closely…the atoms are the true elements of bodies", a statement which is not, in my opinion, correct. The atomic theory can, it is true, contribute enormously to—indeed, may be necessary for—visualising how the basic substances persist in simple substances and compounds; but the concept of basic substance as such does not in itself contain any idea of atomism. It was, after all, while explicitly rejecting atomism that Lavoisier carried this concept to victory; and also in more recent times, there were, and are, chemists who avoid the atomic theory but retain the elements, including, of course, elements in the sense of basic substances (Paneth 1965, p. 133).

After all, to claim that the central mystery of chemistry, namely the question of how elements persist in their compounds, has been fully resolved by the quantum mechanical explanation is to fall into the trap of presentism. I believe it may be more fruitful to keep the philosophy of chemistry alive, as it were, by resisting a reduction of such a philosophical question to protons, neutrons and electrons.[5]

Contemporary similarity studies on the elements

Focusing on the properties of combined simple substances and simple substances has also been the basis for a number of similarity studies carried out by the Colombian school of

[4] This section arose entirely as a result of a reviewer's helpful comments, although I disagree with the reviewer's position.

[5] I would even venture to suggest that maintaining Paneth's 'metaphysical' understanding of the concept of 'element' might allow one to achieve some continuity with the ancient and alchemical notions of elements and compound formation.

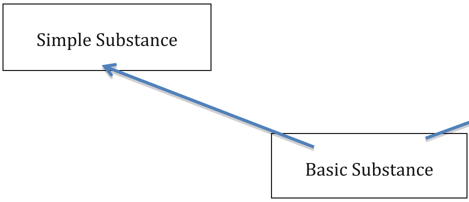

Fig. 2 Proposed clarification for discussion of 'element' concept. Three way relationship whereby element as basic substance underlies both simple substance and combined element. All three terms are confusingly referred to as "element" at least in the English language

theoretical chemists of Jose Luis Villaveces. The first such study was due to the British biologist Sneed who is better known for his work in biological classification. It was Sneath, along with Sokal, who pioneered the use of numerical taxonomy to explore biological classification (Sneath and Sokal 1973). In 2000 Sneath turned this approach to the classification of the elements and obtained some significant results (Sneath 2000). His study consisted of assessing the degree of similarity between 45 selected chemical and physical properties of some 69 elements. Sneath found that elements fell into close clusters reflecting the familiar s, p and d blocks of the periodic table.

He was also able to recover several more specific features of the conventional periodic system such as the strong kinship that exists among the elements in group 1 (alkali metals) as well as among the noble gases. The more recent studies, partly inspired by the work of Sneath, have extended the scope of the earlier studies to examine as many more properties and more elements as simple substances as well as elements in combined simple substances (Restrepo and Pachón 2007).

One interesting extension of this work might be to consider the relative extents to which focusing on properties of combined simple substances as opposed to properties of simple substances can recover important aspects of the periodic system. This might enable one to erode the commonly held view that it is mainly the properties of simple substances that govern the periodic table. It would not however enable one to address the Mendeleev–Paneth claim that it is the elements as basic substances which primarily govern the form of the periodic table.[6]

As is also generally held, it is necessary to also consider elements in combined form, or what I propose to call combined simple substances in order to arrive at the periodic system. I take it that combined simple substances as well as simple substances are at the same epistemological level, as it were, while elements as basic substances underlie both of these forms and therefore exist at a deeper level of nature. The following diagram is intended to clarify this relationship (Fig. 2).

What is the periodic table?

I come to the second question in my title. The easiest way to explain what the periodic table is, would be to do the following. If the elements are arranged in order of increasing

[6] As a matter of fact it is not entirely clear that Mendeleev ever made the claim about elements as basic substances that Paneth attributes to him and that has been largely taken for granted by contemporary philosophers of chemistry who have written on this topic.

H																														He
Li	Be																								B	C	N	O	F	Ne
Na	Mg																								Al	Si	P	S	Cl	Ar
K	Ca														Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr														Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Th	Pa	U	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn						

Fig. 3 Long-form periodic table. Each period lengths show a doubling except for the very first period consisting of two elements

atomic number, approximate repetitions, or periodicity, occurs every so often in this linear sequence. The interesting feature about chemical periodicity is that the interval between successive periods shows a variation as atomic number increases. In addition the period lengths show a doubling in most cases. The sequence of period lengths is as follows, 2, 8, 8, 18, 18, 32, 32… The behavior observed in all periods apart from the very first one has been called 'period doubling' and it continues to be an object of theoretical exploration as will be discussed in the next section (Scerri 2007) (Fig. 3).

What has quantum mechanics done for the periodic table?

Before addressing this question directly I need to discuss an important point. The application of quantum mechanics to the periodic table represents a reductionist approach with the inevitable result that the focus of interest shifts from macroscopic elements to the atoms of the elements. The modern periodic table is discussed almost exclusively in terms of the periodic table of the atoms of each element. Moreover attention is restricted further to the ground states of the neutral gas phase atoms of the elements which as all chemists agree have little bearing upon the way that these atoms are bonded together in compounds or even within simple substances such as the lattices of diamond or graphite.

The reduction of the chemistry of the elements to the properties of the gas phase neutral atoms has brought about some undeniable benefits in such fields as atomic spectroscopy and chemistry in general but it has also left some questions unanswered. It is to some of these questions that I now want to turn.[7]

For example, there are a number of elements whose placement in the periodic table have been debated by generations of chemists. These elements include hydrogen, helium, lanthanum, actinium, lutetium and lawrencium (Atkins and Kaesz 2003; Cronyn 2003; Dash 1963, 1964; Sacks 2006; Jensen 1982; Scerri 2009). The ground state electronic configurations of the atoms of these elements do not resolve these questions contrary to the perceived dogma in chemistry that electronic configurations explain everything about the elements. As a matter of fact the electronic configurations of these elements may render these questions more ambiguous than they would be if macroscopic chemical properties alone were to be considered.

These days the element hydrogen is traditionally placed in group 1 of the table because it possesses one outer shell electron. Over the years authors have varied among those who would place the element in this group because of its ability to form H^+ ions, or group 17 because of its tendency to form H^- ions (Dash 1963, 1964; Sacks 2006). Some periodic

[7] Another question that I claim quantum mechanics has not clarified is the nature of elements in the fundamental sense discussed in the earlier parts of this article.

table designers avoid this ambiguity altogether by allowing hydrogen to float above the main periodic table in a rather unique fashion, sometimes accompanied by helium but not always (Atkins and Kaesz 2003).

In the case of helium, the traditional placement is in group 18 or the noble gases in view of the obvious chemical inertness of this element. But with the advent of electronic configurations and quantum mechanics some authors have sought to maximize the agreement between the electronic structure of helium atoms and the periodic table. Supporters of the left-step periodic table favor placing helium in group 2 of the table because of its possessing two outer electrons, despite of its apparent dissimilarity from the alkaline earth metals.[8]

Of course chemists have tended to resist this relocation of helium, a response which incidentally highlights another aspect of the relationship between chemistry and physics in this context. Chemists are happy to embrace reductionism to quantum mechanics and atomic concepts so long as it helps them to rationalize chemical phenomena but when a physical description contradicts the chemical behavior they readily ignore the dictates of physics.

A possible historical analogy?

One can see a certain parallel between the use of electronic configurations to classify elements into groups and the use of atomic weight to order the elements in the original periodic tables devised by Mendeleev and other early pioneers. The use of the latter ordering principle produced a few anomalies called ‘pair reversals’. For example, assuming an ordering based on increasing atomic weight the element iodine should be placed before selenium but this makes little sense in terms of chemical properties since iodine belongs with the halogens and selenium belongs in the oxygen group. The early pioneers of the periodic table simply reversed such pairs of elements in the belief that the underlying basis for the periodic system would eventually show that they were justified in doing so. Such justification duly appeared in the form of atomic number that was postulated by van den Broek and confirmed experimentally by Moseley.

I believe a similar thing is true of the placement of helium. In spite of the dictates of current physics, secondary classification, or the placement of elements into groups, requires that helium be left in group 18. If this is correct, it highlights another deficiency of the reduction to gas phase atoms. As things stand, at the moment, the microscopic criterion for the placement of hydrogen and helium are surprisingly different. We traditionally place hydrogen in group 1 because of the presence of one electron in its electron shell, while we place helium in group 18 because of the absence of one electron, not because of the presence of a certain number of electrons, as is carried out in the case of every other element. This situation is surely less than ideal.

Before moving on, let me mention a recent idea that I have proposed which would actually strengthen the reductionist case in the context of the periodic table. The idea concerns triads of elements like lithium, sodium and potassium. It was the discovery of such triads of elements that provided the first hint of a mathematical regularity underlying the elements. In the case of these three particular elements, and for every other valid triad,

[8] Some even claim that an appeal to the nature of gas phase isolated atoms represents an appeal to elements as basic substances as discussed in the previous section on this paper (Bent 2006).

the middle element of the three simultaneously shows intermediate chemical reactivity as well as having an approximately intermediate atomic weight.

$$(\mathrm{Li} + \mathrm{K})/2 \approx \mathrm{Na}$$
$$(6.941 + 39.098)/2 = 23.019 \approx 22.990$$

As was pointed out above, the ordering principle of the periodic table has now changed to atomic number. It is natural to therefore consider what bearing, if any, this change might have on triads of elements. As it emerges, those triads which are approximate when using atomic weights become exact. This occurs simply because atomic numbers are whole numbers unlike atomic weights.

$$(\mathrm{Li} + \mathrm{K})/2 = \mathrm{Na}$$
$$(3 + 19)/2 = 11$$

Based on this encouraging feature I have suggested trying to increase the number of atomic number triads and thereby possibly resolving some or all of the long-standing issues to do with the placement of elements (Scerri 2009). Let me first give one example of this. If hydrogen is relocated to group 17 then one obtains an exact atomic number triad ((H + Cl)/2 = (1 + 17)/2 = 9). Similarly this approach confirms the chemical intuition that helium should *not* be relocated from group 18 to group 2.

$$(\mathrm{He} + \mathrm{Ar})/2 = \mathrm{Ne}$$
$$(2 + 18)/2 = 10$$

Whether or not this approach has any fundamental validity or whether it is all numerology has been the basis of some discussion in the literature (Schwarz 2010). I suppose we must wait and see.

Another difficulty for quantum mechanics. Derivation of the $n + \ell$ or Madelung rule

One remarkable success of quantum mechanics when brought to bear on the periodic table, has been the explanation of why different periods can contain 2, 8, 18 or 32 elements. This feature follows naturally and deductively from quantum mechanics. From the solutions of Schrödinger's and Dirac's equations for the hydrogen atom one can rigorously derive the existence of four quantum numbers and the relationship between them.[9]

This scheme rigorously explains why there are be a maximum total of 2, 8, 18, 32 etc. electrons in successive shells as one moves further away from the nucleus. But does the fact that the third shell can contain 18 electrons also explain why some of the periods in the periodic system contain eighteen places? Actually not exactly. If electron shells were filled in a strictly sequential manner there would be no problem and the explanation would in fact be complete. But as anyone who has studied high school chemistry is aware, the electron shells do not fill in the expected sequential manner. The configuration of element number 18, or argon is,

$$1s^2, 2s^2, 2p^6, 3s^2, 3p^6$$

9 Since I have discussed this issue in previous publications I will not do so again here (Scerri 2004).

It is from experimental data that the lengths of the periods are known and not from ab initio calculations. The development of the period from potassium to krypton is not due to the successive filling of 3s, 3p and 3d electrons but due to the filling of 4s, 3d and 4p. It just so happens that both of these sets of orbitals are filled by a total of 18 electrons.

As a consequence the explanation for the form of the periodic system in terms of how the quantum numbers are related is semi-empirical since the order of orbital filling is obtained from experimental data. Consider now the cumulative total number of electrons which are required for the filling successive shells and periods, respectively,

Closing of shells
Occurs at Z = 2, 10, 28, 60, 110 (cumulative totals)
Closing of periods
Occurs at Z = 2, 10, 18, 36, 54, etc.

It is the second sequence of Z values which really embodies the periodic system and not the first. For all we know, electron shells may not even exist or may be replaced by some other concept in a future theory. But the fact that chemical repetitions occur at Z = 3, 11 and 19, if we focus on the alkali metals, for example are chemical facts which will never be superseded.

Only if shells filled sequentially, which they do not, would the theoretical relationship between the quantum numbers provide a purely deductive explanation of the periodic system. The fact that the 4s orbital fills in preference to the 3d orbitals is not predicted in general for the transition metals but only rationalized on a case by case basis. In some cases the correct configuration cannot even be rationalized, as in the cases of chromium and copper, at least at this level of approximation. Again, I would like to stress that whether or not more elaborate calculations finally succeed in justifying the experimentally observed ground state does not fundamentally alter the overall situation.

To sum-up, we can to some extent recover the order of filling by calculating the ground state configurations of a sequence of atoms but still nobody has deduced the $n + \ell$ rule from the principles of quantum mechanics. There have been many attempts to do so but none have been successful (Ostrovsky 2001; Bent and Weinhold 2007; Allen and Knight 2000).[10] Perhaps this should be a goal for quantum chemists and physicists if they are really to explain the periodic system in terms of electronic configurations of atoms in ab initio fashion.[11]

[10] Also see a critique of Allen and Knight in (Scerri 2006) and of Bent and Weinhold in (Scerri 2009).

[11] Not everybody agrees that it is the duty of physics to derive or explain the Madelung rule. Some point to its approximate nature in that it appears to show about twenty exceptions, namely the anomalous electronic configurations starting with the atoms of chromium and copper. Others believe that it may first be necessary to explain the Madelung rule via group theory, before turning to a quantum mechanical explanation. They point to the discovery of the omega minus particle which was predicted by Gell-Mann and Ne'eman by the use of group theory well before a quantum mechanical explanation of quantum chromo-dynamics. One such proposal comes from Pieter Thyssen who is actively seeking such a group theoretical understanding of the Madelung rule (unpublished talk at 2011 meeting of ISPC in Bogota, Colombia). He is part of a long-standing tradition of group-theoretical work mainly carried out in the former Soviet Union.

Possible response from physics and conclusion

One kind of response that one sometimes hears from physicists, to the kinds of problems that I have raised, goes something along the following lines. The periodic table is in any case an approximate scheme from classical chemistry and the fact that some of its features cannot be deduced from quantum mechanics is not therefore of any great consequence. They believe that the periodic table, or the periodic law is a level specific law which is eliminated in the act of being reduced to physics, in which case it is futile to even ask such questions.

But such a response completely misses the point. It would be like saying that the question of the reduction of life itself can be eliminated by realizing that living systems are made of certain components like amino acids, DNA, proteins and so on and that their chemistry is known to obey the laws of chemistry and so one should not be making such a fuss. In the case of living organisms it is easier to see the folly in such a response.

The apparent emergence of life out of these fundamental chemical building blocks does indeed appear to be a mysterious phenomenon until one appreciates the role of evolution which has been taking place for billions of years. During this time nature has conducted innumerable experiments with different sequences of DNA, different proteins and so on in such a way that all the apparent intermediate acts of emergence can be explained as the result of natural processes fully dictated by the laws of chemistry.

Similarly, the elements have evolved from atoms that have themselves evolved from the primordial soup of elementary particles. Once the modern elements were in place the rather mysterious relationship, that we know as chemical periodicity, came into being whereby after every fixed sequence of elements is traversed there occurs an apparent repetition in chemical properties. The gap from quantum mechanics to chemical periodicity may not be fully bridgeable as things stand at present but there is no need to invoke emergence just as there is no need to invoke the emergence of life from inanimate molecules like DNA and amino acids. It is not that chemistry is ontologically irreducible to quantum physics but only that it is currently epistemologically or theoretically not fully reducible.[12]

Given that chemistry and physics have only been seriously practiced for something like 500 years, and given that these two fields have developed largely independently, it is hardly surprising that there is an apparent lack of theoretical or epistemological reduction. Meanwhile attempts to show that chemistry is ontologically non-reducible to quantum mechanics or that chemistry emerges or that there is downward causation from chemical to physical levels are entirely unconvincing at least to the present author (Hendry 2010). But to put my case against emergence in chemistry would require an entirely different paper (Scerri 2012). I have also made a start in a recent editorial for this journal (Scerri 2011).

My own research has examined the reduction of chemistry to quantum mechanics and I have pointed out the limitations in the claims that this reduction is full and complete. However, in the light of more extreme and unqualified anti-reductionist claims made by others in the field I find myself also increasingly stressing the extent to which the reduction has been largely successful (Scerri 2007, 2008).

[12] My brief mention of reduction and emergence may not be sufficiently sensitive to the range of positions that these terms have been taken to represent. This is not the place to enter into a review of the large literature on these topics. I do however want to suggest that the relationship between the periodic table and quantum mechanics is a fertile ground for these more general philosophical debates.

The question of whether or not chemistry has been reduced is not a black and white or yes–no question. It is more about the degree to which reduction has been achieved. I believe that philosophers of science who have concluded that reductionism fails in the case of chemistry to physics are mistaken. But such claims appear to be as much a criticism of the logical positivist stance on reduction rather than an examination of the detailed facts about chemistry and quantum mechanics. This is an unfortunate situation which is nicely offset by the work of such philosophers of science as Alan Chalmers whose organizational efforts produced this excellent symposium in Sydney.

To return to the title of my paper, I must conclude that while attempts to reduce chemistry to quantum mechanics have clarified a number of issues and have brought tremendous advances, they have failed to cast any substantial light on the essentially philosophical question of the fundamental nature of elements.

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