How Much History Can Chemistry Take?

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Abstract: Chemistry is typically considered to be a nomothetic science, *i.e.* a science interested in general laws rather than historical facts. Also, the unification of science is usually envisioned as an effort to connect particular scientific disciplines through their laws, *e.g.*, the laws of chemistry are to be derived from the laws of physics. It is however equally sensible to combine the sciences through a single cosmic history. There is a large literature following this direction, albeit rarely focused on chemistry. In this paper some ideas concerning the possible role of a 'historical' (or 'idiographic') chemistry are presented, with special attention to the notion of a 'genetic' classification of chemical compounds, and to the counterintuitive proposition that many major branches of physics may in fact be explained by chemistry, not the opposite.

Keywords: *Astrochemistry, geochemistry, classification of chemical compounds, nomothetic and idiographic sciences, unification of science.*

1. Introduction

The Kantian philosopher Wilhelm Windelband (Windelband 1894) developed a distinction between idiographic and nomothetic sciences. Simply put, idiographic sciences aim to discover and describe the unique history of the world, while nomothetic sciences are interested in general laws, applicable to any fact of a given type, regardless of its spatiotemporal location. A paradigmatic science of the first sort would be the history of human civilization, but also evolutionary history, paleontology, or any other branch of science as long as it discusses individual facts that have their specific place in the wider history of the world and will not happen again. Typical nomothetic sciences include the various disciplines of physics – from quantum mechanics and fluid dynamics to the theory of crack propagation – but also the synthetic theory of evolution, geodynamics and, last but not least, chemistry.

Chemistry is traditionally considered to be a typical nomothetic science – interested in finding general laws applicable to the amazing complexity of the chemical world, and organizing the chemical lore with a limited set of funda-

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mental laws. It is visible in university-level textbooks (*e.g.* Pauling 1988, Miessler & Tarr 2010), introductory-level courses (Corwin 2007), pedagogical theory (see *e.g.* the concept of 'chemical logic' in Jakubowski & Owen 1998) and original research on the foundations of chemistry (*e.g.* Boeyens 2008). Basically, all these sources agree on one thing: what is really important in chemistry is a certain basic set of first principles, and as soon as you have mastered them, everything will be made clear. It is the very essence of nomothetic thinking.

The purpose of this article is to examine the possible place of chemistry in the wider panorama of the 'pan-idiographic' science of the history of the Universe, a science proceeding to describe the unique history of the world: from the Big Bang through the astrophysical and geophysical processes up to the realm of pre-biotic and biotic evolution. It is proposed that there might be more hope to create the 'pan-idiographic' than the 'pan-nomothetic' science in the foreseeable future, and that chemistry would play a critical role in its structure.

2. What is the problem with a 'pan-nomothetic' science?

Ernest Nagel proposed in *The structure of science* that a science B is reduced to science A if all of the fundamental concepts of science B may be defined in the language of science A (Nagel 1979). For the purpose of this article, the term 'pan-nomothetic science' will denote a hypothetical science based on fundamental physics, performing a series of reductions *sensu* Nagel to derive all other nomothetic sciences. Such a science is often envisioned as the end-goal of the scientific endeavor (*e.g.* Weinberg 1994), and although a general scheme of such a chain of reductions is known, there are gaping holes in the picture, some of them proposed to be not repairable. The old philosophical problem of emergence (Alexander 1920) is based precisely on the notion that at certain points a reduction of science B to science A is impossible, because a certain property of the objects described by science B is *a priori* irreducible to properties of any 'lower-level' science A. A typical example is the proposed irreducibility of biology to any lower-level science (Mayr 1997, p. xvi). It is beyond the scope of this article to discuss the problems of theoretical reduction in detail. However, it would be instructive to note few objections commonly raised against reduction scenarios involving chemistry. It might be a good starting point to consider the reasons to develop the pan-idiographic science and the 'historical chemistry'.

The derivation of the properties of molecules from quantum mechanics (QM) is widely recognized as a successful and promising development. More careful analyses however often point out that for physical systems of any reasonable complexity, certain techniques of approximation have to be employed – which puts in question the ability of QM to form a 'strict' reduction base for molecular chemistry (*e.g.* Ostrovsky 2005, Boeyens 2008, p. vi). A typical example is the use of the Born-Oppenheimer approximation (BOA) in quantum chemistry calculations. Although the error caused by the fixation of nuclei is small enough to make QM useful in calculations of molecular structures, the use of BOA it certainly not the kind of development that could be equated with 'straight' reduction. Other authors have noted that regardless of the success of QM in explaining certain chemical laws, in everyday chemical work other, non-reductive methods are used, such as Lewis structures or the VSEPR theory and that closer inspection of the proclaimed paths of reduction reveals in fact much incompleteness (Scerri 2007).

The proposition here is that, generally, there is a serious problem with the reductive model and, by transition, there are serious obstacles to having a rigorous 'pan-nomothetic' science in the foreseeable future. Let us rephrase the main problems.

On the one hand, the millions and billions of individual components, each complex in its own, have to be taken into account in any reductive model. And although it is sensible to 'drop' certain terms of equations for practical needs, it is not possible to do it for the purposes of theoretical reduction. On the other hand, we should consider for a moment what is the point of performing reduction in the first place. It seems that for the purposes of forwarding our understanding of nature it is absolutely sufficient to know the overall 'roadmap' of reduction only: we might be content that it seems the theory of electronic states of complex molecules is 'in principle' derivable from quantum principles, while it would be madness to use 'straight' QM every time we need to predict the migration of electrons in interacting proteins.

It would also be interesting to ask, would it *really* be psychologically satisfactory to derive, say, the behavior of lipid membranes from QM. Suppose that some stubborn quantum chemists, using weeks of computation time, actually predicted the segregation of cholesterol-based lipids into rafts in a lipid bilayer. *How* exactly would that count as a reduction of lipid membrane thermodynamics to QM? Would a printout of 10^{15} binary operations suffice?

Going even further, one may wonder, can such a reductive pathway work as an explanation of *the real world*? Pure mathematical physics can easily describe cubic planets, stars made of pure neon or blocks of uranium the size of one cubic kilometer (Hempel 1966) – yet these objects do not exist, because there are no natural processes actually producing them in the course of the cosmic evolution. To make a slightly more subtle point – there seems to be a possibility for stable isotopes with mass numbers around 300 to exist: the so-called 'island of stability'. Yet, as far as we know, there are no such isotopes actually present in the universe. There is no way of explaining that particular fact with nuclear physics only and without the appreciation for the cosmic history and the actual conditions available in the cosmos. Similarly, the early tendencies of explaining the phenomenon of life using solely the theoretical principles of chemistry or physics (Schrödinger 1992) have evolved into more sophisticated attempts that include the knowledge of the actual physico-chemical context for life formation on Earth (Rauchfuss 2008). To sum up – it may be not only for pedagogical reasons (Earley 2004) that a pan-idiographic, historical, or evolutionary context for chemistry is needed.

3. So what is the alternative?

It is not the purpose of this paper to undermine the attempts to create a 'pan-nomothetic' science. The previous part was rather intended to show that chemistry, while standing in a central place of such a science, is at the same time a testing lab for all of the difficulties related to the reductionist, 'pan-nomothetic' program. This 'negative' introduction is not without its 'positive' counterpart. I believe that the traditional, automatically assumed nomothetic view of chemistry is partly responsible for the general lack of chemists in the ongoing creation of a 'pan-idiographic' science. What is meant by that name?

The 'pan-idiographic' science is, simply put, the science of the history of the universe. Its goal would be to combine the sciences by the 'unity of history', not by the 'unity of laws'. It would unfold, it seems, in two related strands: top-down and bottom-up. First, with physical cosmology of the Big Bang, followed with galactic, stellar, and planetary system astrophysics, and up to geophysics and various branches of geology. Second, it would discuss particle and atomic physics (but be concerned rather with specific loci of nucleosynthesis rather than calculation of theoretical cross-sections), and later become nothing more than a sort of 'historical chemistry', also 'historical mineralogy', prebiotic chemistry, and history of life on Earth.

Similar concerns have been raised by several authors (*e.g.* Haken 1978, Earley 2004, Vihalemm 2001, 2005, Näpinen 2007). Both Vihalemm and Näpinen advocate openly for the introduction of *history* into chemistry, for reasons of their own. Vihalemm attacks the problem from the point of view of philosophy of science and describes chemistry as "a research field with a dual character" (Vihalemm 2005, p. 175) – a science interested in *constructing* *laws* (a "phi-science"), yet at the same time interested in *particular chemical substances* "regardless of the fact whether and to what extent this is possible on the basis of the laws of nature" (Vihalemm 2005, p. 175). He points to numerous consequences that would be brought by the adoption of a new philosophical basis for chemistry; here I would rather discuss the importance of a similar conceptual shift for the science of chemistry itself and its relations to other natural sciences. Näpinen, on the other hand (Näpinen 2007), uses a particular example of the science of non-equilibrium thermodynamics as a leverage point and introduces the contrast of *organization* and *self-organization*, based on the well-known work of Prigogine (*e.g.* Prigogine 1997) and his co-workers.

The influential paper by Earley (Earley 2004), although revolving around the problem of education, is probably the closest to my perspective on the issue. The change that is advocated in Earley's paper is described as a shift from an *analytical* to a *synthetic* approach to chemistry. The synthesis would be historical in nature:

> The old story-line of introductory chemistry courses – 'whatever exists can be understood through *analysis* into its component parts' – is no longer sufficient. A more appropriate story-line would be – 'everything came to be through *synthetic* processes' – that is, the Evolutionary Epic. Perhaps we should start with some remote situation, and tell a connected, coherent story of how the world came to be as it is – a story that *ends up* where the students live. Logically, perhaps one should start with *the vacuum* – an excitable medium. New classes of entities – quarks, atoms, molecules, stars, organisms, societies – could then be introduced as arising in evolutionary (historical, in Collingwood's sense) transitions from prior entities. [Earley 2004, p. 149]

It is interesting to see how everybody seems to be describing the same paradigm shift, yet there is a bewildering variety of terms used to describe it; I use the pair 'nomothetic – idiographic' simply because it has a historical flavor that I enjoy. It does not seem to be inherently better than a pair 'phi-science – natural history' or 'organization – self-organization' or 'analytical – synthetic'. The names are not important. What I believe should be done is a consideration of how would that paradigm shift work *in practice* – how would it influence the science of chemistry and other sciences that are intimately related to chemistry.

In the following chapters, I shall use the example of classification systems to illustrate some problems with the realization of the philosophical proposition discussed here, and later argue for some conceptual developments that may results from the work on 'historical chemistry' in the context of the 'pan-idiographic science'. In my opinion, the first part shows just how terribly difficult in practice it is to apply standard methods of an idiographic science to chemistry, and the latter – how big the payout may be.

4. Towards a ‘natural’, genetic classification of chemical species

The traditional classification of chemical species is by structure. Nuclei and their isotopes are classified by the numbers of nucleons; atoms by their electronic configuration. There are many competing classifications of chemical molecules and most of them make use of a certain morphological criterion – the presence of rings (aromatic versus aliphatic hydrocarbons), the type of bonding (alkanes versus alkenes versus alkynes), the number of monomer units in polymers (dipeptides, oligopeptides, proteins), the polarity of the molecules (hydrophiles, lipophiles) *etc.* Classification criteria of that sort often lead to apparent paradoxes, because most large molecules include functional groups of various kinds – hence the concepts such as amphiphilic molecules or zwitterions. Current systems of classification are extremely well developed, but the need to keep a discrete system in the light of the non-discreteness of nature’s chemical creativity results in somewhat arbitrary definitions, like the IUPAC’s non-inclusion of cyclitols to the group of carbohydrates (McNaught 1996). That is however the sore of all ‘structural’ classification systems, *i.e.* systems based solely on the objects’ inherent properties, not on their history. As the purpose of this article is to examine the possibility of a ‘historical chemistry’ that is an organic part of a wider ‘pan-idiographic’ science, it might be helpful to mention one example from a neighboring discipline. The history of biological classification is a beautiful example of how a seemingly simple system turns out to be a nightmare in the light of the real complexity of nature. Let us consider the example of plants.

The straightforward definition of plants as multicellular organisms performing photosynthesis would currently lead to the inclusion of not only the paradigmatic land ‘green plants’ (currently grouped as embryophytes), but also rhodophytes and chlorophytes plus certain more cryptic and evolutionarily unrelated entities like brown algae and water molds. The resulting consensus definition is exceedingly unintuitive: the so-called true plants (*Viridiplantae*) are in one oft-cited source circumscribed as “platycristate taxa with or without flagella, with chloroplast containing chlorophylls *a* and *b*, eyespot when present in plastid, basal bodies anchored by cruciate system of rootlets” (Patterson 1999). Every bit of information is needed, because in the course of evolutionary process various forms of photosynthetic organisms evolved, sometimes transmuting via convergent evolution into forms differing from ‘true plants’ only by minute ultracellular (like the form of mitochondrial cristae) or biochemical (like the variation of chlorophyll) features.

It is however only at the level of ‘synchronically’ considered structure that these differences may seem minute and the abovementioned definition unnecessarily detailed or arbitrary. If analyzed diachronically – in the context of the universal tree of life – plants form a nicely diverging, monophyletic taxon with its own particular history, relatives, and resulting derived characteristics (synapomorphies). It is becoming more and more popular to define *all* taxa phylogenetically (Mayr 1997). It is now a cliché that living organisms should not be classified according to 'skin-deep' similarities, but according to family relationships: nobody seriously considers grouping bats, birds, and pterodactyls (or snakes, earthworms, and caecilians) just because they are similar. It might be interesting to examine how a similar point of view would apply to the science of chemistry. Also, the 'historicization' of chemical classification systems would automatically bring us much closer to the unification of sciences. If we really want a 'historical chemistry', than we also need a 'historical classification system': just like evolutionary biology needs a phylogenetic taxonomy.

5. The work done so far

I am aware of only three areas in the scope of chemistry broadly understood in which the program of 'historical' (or 'genetic') classification has been developed in considerable detail: the classification of isotopes (in the context of nucleosynthesis), of certain small molecules (in the context of astrochemistry), and of minerals (in the context of Earth system evolution). The following three chapters will be devoted to the concise description of these examples. The discussion of their philosophical significance will follow.

5.1 Nuclei and atoms

The traditional, logical classification of atoms is the periodic table – combining the 'numerical' enumeration of nuclei according to the number of protons with the vertical arrangement of the table according to the filling of subsequent electronic shells. An amazing amount of information can be read out of this simple scheme. What would then be a 'genetic' classification of elements? The history of any atom goes back to a certain event of nucleosynthesis, and there is now a considerable agreement as to the genesis of atomic species present in the universe. These are typically tied to specific sites of nucleosynthesis (BB, stellar hydrostatic, stellar explosive, *etc.*) or to specific modes of nucleosynthesis (alpha particle addition, s- and r-process nucleosynthesis, *etc.*). The resulting agreement (see *e.g.* Burbidge *et al*. 1957, Wallerstein *et al*. 1997) is that from the point of view of the mode of generation, there are only few major groups of elements:

- 'primary' elements formed in BB nucleosynthesis: H, Li, and He;

- ‘secondary’ elements formed after BB:
    - elements forming in hydrostatic stellar burning: most elements up to the ‘iron peak’, including C, O, Ne, and Mg;
    - elements forming via slow neutron capture (the ‘s-process elements’): much of the elements past the iron peak, notably Sr, Y, Zr, Ba, La, Ce, Pr, Nd, Pm, Sm;
    - elements forming via rapid neutron capture (the ‘r-process elements’): approximately the other half of the heavier nuclei, notably the vast majority of As, Br, Rh, Ag, Sb, I, Cs, Eu, Gd, Tb, Ho, Re, Ir, Au, and all of the elements with atomic number Z higher than 83 (s-process nucleosynthesis does not proceed past $Z = 83$).

In addition there are other minor groups, such as the group of light elements formed by the so-called x-process, notably boron. Also, it should be noted that the classification scheme above is simplified for the purposes of clarity: in reality, all nuclides, not just elements, should be discussed.

In contrast to this widely discussed area of nuclear chemistry, one interesting project pursued by a single scientist should also be mentioned here: the ‘Earth Scientist’s Periodic Table’ devised by B. Railsback (Railsback 2003). This periodic table is a proposition to group elements (or rather, their ionic states) by charge, and further, by properties that result in a different overall geochemical behavior. For our purposes, the author’s philosophical remarks are even more interesting. Railsback claims that:

> the conventional periodic table is product of Platonist-idealist thought: the elements are considered only in an ideal state, and each element has only one perfect condition/position. This Platonist view ignores the fact that many elements don’t exist in nature in this purportedly ideal (uncharged) state, and that many elements exist in multiple charges or states. The new table acknowledges that natural reality deviates from ideality, and that things take different character under different conditions. [Railsback, electronic document]

Effectively, the table is not that different from the ‘ordinary’ table, but it is clearly designed to show what various elements ‘do’ and ‘where do they come from’ (the ‘idiographic’ flavor) rather than to group them in an abstract state space (the ‘nomothetic’ flavor). It is possible to read out of the diagram which elements are incorporated in primary magmas, which elements are abundant in seawater, which are essential for life, *etc.*

5.2 Molecules of astrophysical concern

The literature on the chemical evolution of the universe is vast and detailed (for a review, see *e.g.* Herbst 2001). There is only a handful of confirmed gas-phase chemical species in interstellar matter (ISM), with all of the more complex ones occurring only in so-called molecular clouds: structures of dense interstellar gas where the low temperature and shielding from UV radiation allows the formation of larger molecules. Additionally, a large variety of molecules and supramolecular structures, notably polycyclic aromatic hydrocarbons (PAHs) and their aliphatic modifications, are suspected to occur on the surfaces of interstellar grains. The general picture is that first molecules, usually simple diatomic species like CO, form in the outer envelopes of dying stars, then follows their evolution in ISM, and the next significant boost to the chemical complexity of the universe occurs in the protoplanetary disks where higher concentrations and effective radiative shielding allow more diverse reactions to proceed. Astrochemists in their work typically group molecules according to environments in which they are abundant – a different mix is to be expected in the gas phase of diffuse interstellar clouds, in molecular clouds, and in interstellar grains as well as on their surfaces (Shaw 2006) *etc.*

One interesting fact that may be mentioned here is the suspected dependence of interstellar H_2 on the presence of grains (Shaw 2006, p. 131) related to the fact that the simple H + H association in the gas phase seems to be forbidden by the lack of energy levels of free H_2 necessary to radiatively stabilize the molecule. This leads to the surprising hypothesis that, at the galactic scale, H_2 is essentially a 'solid-state molecule' which means that most of molecular hydrogen comes from the surfaces of solid bodies. This, again, is not something that we would predict based solely on quantum mechanics.

5.3 Mineral evolution

In the sea of relevant papers, one particularly enlightening review is called simply 'Mineral evolution' (Hazen *et al.* 2008). The paper follows the complexification of the mineral repertoire of terrestrial planets from the ca. 60 species present in the early protoplanetary nebula to the ca. 4300 recognized today. It is admittedly only marginally relevant to chemistry *sensu stricto*, but one crucial point made by the authors makes it worthwhile to consider this paper nonetheless. At the end of the review, its authors describe how structurally analogous mineral species, commonly lumped together in classification systems, are in fact completely unrelated 'genetically'. Specifically, the garnet group of silicates is shown to consist of mineral species occurring in completely different geological settings: grossular ($Ca_3Al_2Si_3O_{12}$) being formed in thermally altered meteorites from the earliest phases of planetary system evolution, pyrope ($Mg_3Al_2Si_3O_{12}$) forming in great pressures and moved to the surface of the Earth by early volcanism, and spessartine ($Mn_3Al_2Si_3O_{12}$) associated with uplifted metasediments, requiring then at least one cycle of rock alteration.

The authors themselves do not put forward a classification scheme explicitly, yet they present a table where specific phases in Earth evolution are related with specific minerals (Hazen et al. 2008, p. 1694), *e.g.* the phase of planetesimal thermal alteration with albite, feldspathoids and biopyriboles; the phase of granite formation with quartz, alkali feldspar, micas, and others; the phase of plate tectonics-related hydrothermal activity with sulfides, selenides, arsenides, *etc.* It is clearly visible that these groupings cut across traditional mineral classes, yet in the historical framework suggested in the paper seem logical and well justified.

Hazen *et al.* (2008, p. 1714) conclude that "mineral evolution complements more traditional approaches to teaching mineralogy by providing an historical narrative for each mineral phase". At the same time most modern textbooks on mineralogy and petrology boldly declare that they present principles rather than facts (*e.g.* Philpotts & Ague 2009).

6. The analysis of these examples

Let us first gather some common features of these examples. First, all of the classification schemes are 'secondary' options; in each case there is a widely accepted alternative, based on a 'structural' principle. The elements are commonly classified by the atomic number or by the electronic state of the neutral species, not by their nucleosynthetic past or geochemical provenience. 'Astrophysical molecules' are not commonly treated as an entity at all and distributed among relevant chemical groups: polycyclic or aliphatic hydrocarbons, metal oxides, *etc.* Minerals are not typically classified by history or tectonic occurrence, but by chemical provenience (silicates, sulfates, oxides, *etc.*), later by structure (nesosilicates, sorosilicates, *etc.*).

Second, all of the propositions mentioned tend to frame a given group of objects in their 'historical' context and allow for a wider look at their place in the history of the universe. The abovementioned 'cosmochemical' classification of isotopes is organically tied up to the theory of stellar evolution, so that the representatives of a given group might be used as indicators of the processes going on in a given astronomical location. For example, the presence of r-process elements suggests the occurrence of supernovae explosions which is in turn tied up to wider, galaxy-scale processes like surges of star formation in encountering galaxies (*e.g.* Springel 2000). This is exactly why such a classification system might be called a 'natural' one. In contrast, there is nothing cosmologically special about, say, a group of chalcogens as contrasted to halogens. This of course is not something new in geology, and mineral species are commonly treated as indicators; the work of Hazen et al.

simply uses this fact to argue for a general historical framework for mineralogy.

Third, all of them are strongly context-based. There may be nothing 'astrophysically special' about chalcogens, and the use of this name in the context of astrophysical nucleosynthesis makes no sense. On the other hand, that category begins to be more 'naturally justified' at the level of mineralogy or biochemistry, where a different overall behavior of chalcogens in contrast to halogens justifies the need for this particular categorization.

Fourth, all of such classification systems include fuzzy categories. This in turn shows that nature often creates no neat family trees, but rather networks of relationship. We may reasonably expect that different paths of chemical synthesis located in completely different environments may produce the same molecules. What it means in practice is that there is no hope for a neat, crisp classification system like the 'structure-based' ones described earlier. Only at the level of systems as complicated as biological systems, we could hope for a large enough number of elemental configurations so that there is no sensible probability that two *identical* objects would form at two different zones of the family tree.

At the very least, the molecules of DNA have sufficient length that it would be nearly impossible for nature to duplicate the same sequence of nucleotides in unrelated populations. Most chemical species consist of tens to hundreds of atoms; even assuming that any configuration of atoms is possible, there is little chance that neat 'family trees' will be discernable, in which certain brands of, say, amino acids would only form on interstellar grains, and others only in aqueous systems on terrestrial planets, with their chemical 'children' (like oligopeptides) also limited in occurrence to these locations. As this is the most serious problem of the whole idea of 'genetic classification systems' in chemistry, some points regarding this fuzziness are worth discussing.

7. Some remarks on the fuzziness of genetic classes in chemistry

There might be a level of fuzziness which makes the whole idea of classifying chemical species according to their history pointless. It occurs where the fuzzy distribution of molecules makes it impossible to predict *anything* using the genetic classification system in question. For example, if it turned out that chemical species of a certain sort occur throughout the universe in more or less equal concentrations regardless of specific physical conditions, it would be impossible to tie their occurrence to any large-scale historical process – the way in which element abundances were shown earlier to be tied to astrophysical processes or mineral abundances to tectonic processes.

How seriously should we consider this threat? I believe that it is much too early to judge. I do not think that we are in a comfortable position to discuss whether derivatives of, say, pyrrole, form a coherent 'family group' tied up more or less tightly with a certain cosmological/geological/biological setting. So the question is, whether an observation of a spectroscopic signature of pyrrole in a patch of night sky would give us some unambiguous (or at least highly statistically significant) information on what kind of a context should we expect to be weaved around those far-away molecules and what other molecules are to be suspected there. The problem is complicated by the very nature of chemistry: there are usually multiple pathways of synthesis and the final product 'has no memory': all traces of its history have been erased. Pyrrole may be formed from other heterocycles, but also from mucic acid and thus ultimately from sugars. This is in stark contrast to the situation in biology. While it is true that there may be multiple evolutionary pathways to photosynthesis or to the formation of the eye, the traces of individual histories are always retained. Molecules, on the other hand, have very little substructure that could help us in deciphering the circumstances of their formation, and elementary particles have absolutely no such substructure.

On the other hand, chemistry also studies large macromolecules and long-chain polymers as well as the still mysterious realm of prebiotic chemistry. Somewhere between the cosmic omnipresence of carbon monoxide or ethane and the cosmic uniqueness of *Escherichia coli* lies the border we are interested in. In other words: where is the point where it becomes feasible to track 'chemical histories'? After all, the purpose of classification is to provide a convenient language. It would then make no sense to create a classification system that satisfies some fancy philosophical urges – for example the need to form groups based on common history – but would otherwise be totally useless. There is however at least one way to deal with this issue.

If it turns out that there is so little regularity in the occurrence of chemical species, that the 'chemical family tree' would be a proposition less than practical, there would still be a place for the examination of 'reservoirs'. Natural processes tend to produce different species in different amounts; similarly, the cosmochemical classification of elements describes in fact the production of differing *mixes* of elements in different environments. The notion of reservoirs is widely used in astrochemistry, but also in geophysics, where different mantle reservoirs are responsible for the production of different suites of igneous rocks (Tackley 2007). The shifting of attention to the generation of differing statistical ensembles by various natural processes is nothing more than an agreement to an even more statistical view of the 'pan-idiographic' science. What would then differentiate among the various settings would be not the *presence* or *lack* of certain molecules or chemical pathways, but rather the *proportions* in which they are present. As a limiting case, some of these species could serve as markers, if the proportion at a given setting would account for the 100% of the occurrence of that species. The presence of PAHs would then mean either interstellar grains or anything else, including cigarette smoke; the presence of large concentrations of acetylsalicylic acid, on the other hand, would unambiguously point to, well, fevers.

Furthermore, such a phylogenetic classification of chemical reservoirs would also automatically direct the attention to the evolution of chemical reaction networks and processes. For example, the formation of stars creates zones of strong UV radiation in the interstellar medium, called photon-dominated regions (PDRs). A characteristic suite of photochemical reactions and products is related to PDRs – similar suites may be discussed for other environments, such as interstellar grains, planetary atmospheres, *etc.*

8. From physics to chemistry and back again

A second, much more exciting role for the 'historical chemistry' would be to track the role of certain chemical facts in the development of the cosmic repertoire of physical laws. Let us return for a second to the cosmochemical classification of elements. It is reasonable to suspect that most of the elements are omnipresent in space. The abovementioned classification of nuclei is actually quite fuzzy for all elements with high abundances – which means that most *typical* small molecules may form practically everywhere. Not all molecules however are typical. The formation of Gd_2O_3 would be limited by the presence of gadolinium which is in turn strongly constrained by stellar nuclear processes. It is not that trivial a fact as it may seem – if we would imagine an astrophysical setting that, for a certain reason, does not produce stars with mass exceeding five Sun masses, we might expect no Gd-based chemistry or Gd-based physics there – and there are examples of physical processes that require a given element to occur. Gadolinium, for one, is one of the very few elements that form alloys susceptible to the magnetocaloric effect. It may be thus sensible to suspect the magnetocaloric effect to operate only in those regions of the cosmos where supernovae have recently been exploding – not necessarily an intuitive result, but one that can be sensibly argued for.

Similarly, there are other physical and physico-chemical processes that operate in nature only in a very narrow range of chemical environments: superfluidity is probably restricted to isotopes of helium; quasi-crystalline phases grow only in alloys of aluminum; the glass transition will naturally occur only in certain groups of silicates and in biopolymers; liquid crystals are typically formed by certain organic macromolecules. Also it may be noted that the whole fascinating field of supramolecular structures is usually discussed alongside specific, rare, and well defined pathways of synthesis, *e.g.* crown ethers which were initially synthesized solely from compounds like phenol or catechol.

It might be surprising to see how many relationships between natural processes come to notice when *real*, genetic relationships instead of *ideal*, structural ones are being analyzed. There are chemical processes and reaction networks that initiate great transformations in cosmic evolution and make it possible for other processes to take place. Seen in the historical perspective, chemistry stands at the meeting point between atomic physics and tens of other branches of physics: surface and colloid science, the study of electronic, mechanical and magnetic properties of condensed matter, *etc.* It would be interesting to describe how the evolution of chemical reservoirs sets the stage for the emergence of complex physics of today's universe – an interesting twist indeed after so much talk about the reduction of chemistry to physics.

To give just one more example: according to some astrophysicists, the formation of the first gravitationally bound objects in the early universe – the proto-galaxies and the first stars – depended on the formation of H_2 which at the time was the only coolant available (Bromm 2010). The recent calculations of some critical parameters in the predominant synthesis reaction of H_2 (Kreckel *et al.* 2010) were greeted with great enthusiasm primarily by the astrophysical and cosmological community which needs these numbers to fill a *historical* gap. There is nothing particularly exciting in a refined calculation of reaction constants – unless this particular reaction is of great importance.

Generally speaking, the consideration of cosmic history gives us a much better understanding of the real place of chemistry in the general framework of universal laws and regularities. The world does not unfold in a way that mirrors the traditional scheme of scientific reductions (from elementary particles, to atoms, to molecules, to macromolecules, to metabolic networks, to life) which would justify the traditional 'pecking order': biology explained by biochemistry which is explained by inorganic chemistry which is explained by atomic physics which is explained by particle physics. To the contrary: some chemical facts explain physical facts, and some biological facts explain chemical facts.

9. Conclusion

The point of this article is to suggest that the inclusion of chemistry into a great unification scheme of sciences does not necessarily have to mean quantum chemistry or, generally, the deduction of the laws of chemistry from a set of more fundamental laws and the deduction of some other laws – like the laws of metabolism – from the laws of chemistry. The unification program itself does not have to imply the 'pan-nomothetic reduction'. In fact, great progress has been made in the previous couple of decades in connecting the historical narratives of biology, geology, astronomy, and particle physics. The 'pan-idiographic science' would describe the real, historical relationships between the subject areas of the natural sciences, and prove that a simple picture of 'biology reduced to chemistry' and 'chemistry reduced to physics' is no longer tenable.

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