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CONCEPTS OF EMERGENCE IN CHEMISTRY

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Introduction

Nowadays many philosophers of science would claim that reductionism as a philosophical programme has failed. The philosophical accounts of inter-theoretic reduction encountered theoretical and practical difficulties. It has been argued that examples of successful intertheoretic reductions in science are few and far between. As regards chemistry, many have expressed doubts that a reduction of this discipline to physics can be had.

On the other hand, nowadays almost everyone is a metaphysical naturalist. Chemists and philosophers alike contend that our world does not contain vitalistic chemical essences, spooky chemical souls, or chemical entelechies. They agree that if all the elementary entities that microphysics talks about (e.g., quarks, leptons, gauge bosons, fields, whatever) were to vanish, there would be nothing left: the atoms, the molecules and everything that is composed of them would also vanish. However, if all atoms and molecules were to disappear, the objects that form the subject matter of microphysics will not necessarily vanish; they may persist (e.g., as plasma). This asymmetry is a straightforward consequence of the direction of the composition relation: the objects that form the subject matter of chemistry are composed of the objects that form the subject matter of microphysics, but not vice versa. As a result, the latter may exist even in the absence of the former.¹ In this very narrow and precise sense then, the microphysical domain has ontological primacy over the chemical domain. This is sometimes referred to as “the generality of microphysics”—all events are, or are exclusively composed out of parts which are, microphysical events, and so fall under microphysical laws.²

It is hard to miss the apparent tension between the two claims made in the preceding paragraphs. If chemical stuff is composed of nothing else

¹ Indeed, there was a time in the history of the universe when the objects that form the subject matter of chemistry did not exist.

² See for example P. Pettit (1993, p. 217).

except microphysical stuff, why doesn't chemistry reduce to microphysics? How could the chemical domain depend so strongly on the microphysical domain, yet not reduce to it?

A number of philosophers have provided reasons to think that the said tension is only *prima facie*. On their view, the generality of microphysics and the irreducibility of chemistry can be reconciled if we regard chemistry as emergent. According to the emergentists, all objects are composed—at their most fundamental level—of microphysical objects; however, it would be a mistake to conclude from here that all properties are physical properties; similarly, it would be a mistake to think that if all events are governed by physical laws then all laws must be physical. If emergentism is correct, there are genuine chemical properties and laws that do not reduce to physical properties and laws, although they are dependant upon them.

“Emergence” is a philosophical term of art, with a lot of appeal to philosophically inclined scientists, including chemists. However, the meaning of this term often remains underarticulated and vague. A prominent contemporary philosopher writes:

The term ‘emergence’ seems to have a special appeal for many people; it has an uplifting, expansive ring to it, unlike ‘reduction’ which sounds constrictive and overbearing. We now see the term being freely bandied about, especially by some scientists and science writers, with little visible regard for whether its use is underpinned by a consistent, tolerably unified, and shared meaning (Kim 2006, p. 547).

I don't think that the use of the term “emergence” is or should be reserved exclusively to philosophers. Also, I am quite sceptical that a unified meaning can be achieved for this term, even amongst philosophers. But I think there is a lot to learn if one pays attention to how philosophers—some of them with a chemistry background—have thought about emergence in chemistry. This paper reviews some of the most prominent concepts of emergence that have been offered so far in the philosophical literature about chemistry.

1. What is Emergence?

As Kim noticed, emergentist positions vary from one author to another and therefore emergentism is hard to pin down. However, there is a set of features that many emergentist positions share. Virtually all emergentist positions hold some form of the view that the world consists of a hierarchy of levels or ontological strata (the microphysical, the macrophysical, the

chemical, the biological, the psychological) and each level depends on the previous level, but it is irreducible to it. Properties at a certain level interact to produce properties at a higher level (emergents). The relation between the lower level and the higher level is usually thought to be supervenience: higher-level properties are said to supervene on the lower level properties.³ These higher-level properties (emergents) arise from those at the lower level, but they cannot be predicted on the basis thereof. Emergents are often deemed to have novel causal powers, i.e., they have the capability to produce effects in a way that cannot be anticipated. Sometimes, emergents are said to be capable of downward causation—the ability to influence the basal conditions from which they arise (i.e., the underlying dynamics). Also, sometimes it is held that emergents involve global rather than merely local properties, and thus they arise only when the basal conditions are characterized by a certain amount of complexity. To sum up, emergents are usually characterized as novel, irreducible, unpredictable/unexplainable on the basis of the lower level theory, and on some views, capable of downward causation.

Typically, emergence is correlated with the failure of reduction. Depending on how one construes irreducibility, one ends up with different types of emergence. On the classical account of reduction due to Nagel (1961), one theory is irreducible to another if the laws of the higher-level theory cannot be deduced from those of a more fundamental theory by employing bridge laws connecting the two levels. For example, if there were chemical truths that cannot be predicted (deduced) from quantum mechanics together with the requisite bridge laws, one would say that chemistry is irreducible to quantum mechanics. However, the notion of predictability is ambiguous; it may refer to predictability in principle or to predictability in practice. If we hold a strong notion of predictability (i.e. predictability in principle) then we end up with strong emergence: chemistry cannot be reduced to quantum mechanics even in principle. If we hold a weaker notion of predictability (i.e., predictability in practice) then some weaker version of emergence obtains; in this case, we would say that chemistry is weakly emergent—chemistry cannot be *in practice* reduced to physics.

In chemistry, the following have been considered emergent or irreducible: chemical compounds, molecules, secondary properties of

³ A set of properties H supervenes on a set of properties L if and only if (i) any two objects x and y that have the same L properties will necessarily have the same H properties (though not necessarily vice versa), and (ii) any two objects z and w that differ in their H properties will also differ in their L properties (though not necessarily vice versa).

compounds such as their taste and colour, temperature, phases of matter, phase transitions, the shape of the molecules, atomic structure and properties, periodicity, aromaticity, chemical bond, chemical structure.

2. Early Accounts of Emergence in Chemistry

One of the earliest authors whose views about chemistry could be labelled as “emergent” is J.S. Mill (1806-1873). In *A System of Logic*, Mill talks about a *chemical mode* of causation, which he contrasts with a *mechanical mode*. In the mechanical mode of causation, the effect produced by two causes acting together is the sum of the effects of each cause acting independently. Mill calls this *the principle of composition of causes*, which in his view is akin to the principle of composition of forces in classical dynamics. On this mode of causation, the effect of the two causes acting in conjunction can be predicted deductively, from the effects of separate causes acting separately. The chemical mode of causation, on the other hand, does not obey the principle of composition of causes.

The chemical combination of two substances produces, as is well known, a third substance, with properties different from those of either of the two substances separately, or of both of them taken together. Not a trace of the properties of hydrogen or of oxygen is observable in those of their compound, water. (Mill 1882, p. 267)

In Mill’s view, chemical compounds have properties that are not “the sum” of the properties of their components taken separately or simply juxtaposed, as in a mixture. Besides the example of water, Mill gives the following examples: the sweet taste of sugar of lead (lead diacetate, $\text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2$) is not the sum of the tastes of its component elements, acetic acid and lead or its oxide; the color of blue vitriol (copper sulfate, CuSO_4) is not a mixture of the colors of sulfuric acid (transparent) and copper(II) oxide (black), from which it is produced. Those effects whose properties do not resemble the properties of their causes are called by Mill *heteropathic*; the laws governing the production of these effects are called *heteropathic laws*. For Mill, the laws of chemistry are heteropathic, since they govern the production of substances whose properties do not resemble those of the reagents.

It is unclear whether Mill’s conception of heteropathic laws is really at odds with reductionism. Admittedly, the properties of chemical compounds are not “the sum” of the properties of their components. But why should we expect them to be? A deductive explanation of the properties of chemical compounds in terms of the properties of their atomic constituents

could still be possible even if the manifest properties of these compounds are not “the sum” of the manifest properties of their components. Of course, for Mill such an explanation was out of sight. But as long as such an explanation remains possible in principle, Mill’s brand of emergentism would be classified as weak at best.

Charles Dunbar Broad (1925) also noted the distinction between purely mechanical behaviour and chemical behaviour. According to Broad, chemistry “seems to offer the most plausible example of emergent behaviour” (Broad 1925, p.65). For Broad, a system is emergent if its properties cannot be predicted from a knowledge of the properties of its constituents taken separately or in other wholes, and of their proportions and arrangements in this whole. According to Broad, the emergent properties of chemical compounds cannot be predicted from exhaustive knowledge of the properties of the parts—the only way to learn about them is to study samples of those compounds.

If the emergent theory of chemical compounds be true, a mathematical archangel, gifted with the further power of perceiving the microscopic structure of atoms as easily as we can perceive hay-stacks, could no more predict the behaviour of silver or of chlorine or the properties of silver chloride without having observed samples of those substances than we can at present. (Broad 1925, p. 71)

The same holds true about chemical affinity. According to Broad, we cannot predict that two elements would combine chemically with each other until we perform the reaction. One of Broad’s examples is that of hydrogen and oxygen:

Oxygen has certain properties and Hydrogen has certain other properties. They combine to form water, and the proportions in which they do this are fixed. Nothing that we know about Oxygen by itself or in its combinations with anything but Hydrogen would give us the least reason to suppose that it would combine with Hydrogen at all. Nothing that we know about Hydrogen by itself or in its combinations with anything but Oxygen would give us the least reason to expect that it would combine with Oxygen at all. And most of the chemical and physical properties of water have no known connexion, either quantitative or qualitative, with those of Oxygen and Hydrogen. (Broad 1925, p. 63)

It would seem that Broad’s view of chemistry fits squarely in what we called strong emergence: the properties of a chemical compound (including its ability to react with other chemicals) cannot be *in principle* predicted from the properties of the elements taken separately. According to Broad, this impossibility stems from the fact that the laws of chemistry

are “unique and ultimate” (Broad 1925, p. 65). By this, Broad means that they are not special cases which arises through substituting certain determinate values for variables in a general law which connects the properties of any chemical compound with those of its separate elements and with its structure. This, in turn, is due either to (i) the existence of innumerable “latent” properties in each element, each of which is manifested only in certain conditions, or (ii) to the lack of any general principle of composition, such as the parallelogram law in dynamics, by which the behaviour of any chemical compound could be deduced from its structure and from the behaviour of each of its elements in isolation (Broad 1925, p. 66-67).

Let’s consider the first possibility. According to a plausible interpretation of Broad, an emergent whole possesses force-generating properties of a sort not possessed by any of its parts (McLaughlin 2008, p. 41). When particles arrange themselves in certain configurations, new forces arise; these have been called *configurational forces*.⁴ In chemistry, configurational forces are higher-level chemical forces characterizing the compounds, irreducible to lower-level physical forces characterizing the components. They are responsible for the existence of emergent behaviour (chemical affinity, the properties of the compounds). Configurational forces are contrasted with *resultant forces*, i.e., non-emergent forces that are the generated by other forces, not by configurations of particles; “emergence”, therefore, is contrasted with “resultance”.

If the second possibility obtains, one cannot learn about the properties of a compound by substituting certain values of the variables in a general law which connects the properties of that compound with those of its constituents, for there is no such general law. This would explain why the trans-ordinal laws that connect the properties of the atoms with those of compounds are *unique* and *ultimate*. They are *ultimate* because in determining the properties of a chemical compound there is no theoretical shortcut, one must study a sample. They are *unique* because by studying the rule Nature follows when it produces a certain compound one cannot learn anything about the rule Nature follows when it produces other compounds.

Is Broad’s emergentism weak or strong? Given Broad’s “mathematical archangel” metaphor, one would think that Broad’s emergentism is of the strong kind. But caution is required if we try to establish whether or not on

⁴ Although Broad does not use this term, McLaughlin (2008) interprets Broad in this way. According to McLaughlin, “it is clear that he [i.e., Broad] maintains that certain structures of chemical compounds can influence motion in fundamental ways” (McLaughlin, 2008, p. 47).

Broad's view chemistry is strongly emergent. Broad was aware of the possibility that the laws of chemical combination and the properties of compounds could turn out to be mere consequences of the laws of microphysics (Broad 1925, p. 73). Indeed, it has been argued that the advancements in the understanding of the atomic and molecular structure that took place during the 20th century make Broad's claims regarding emergence in chemistry implausible (McLaughlin 2008). If these arguments are sound, Broad's emergentism may be strong, but chemistry is not an example of strong emergence.

3. Contemporary Accounts

A recent approach to emergence in chemistry is due to Hendry (2006). Hendry's account is based on the classical notion of emergence advocated by Broad. Hendry does not accept McLaughlin's conclusion that there is no scintilla of evidence that there are configurational forces or downward causation in chemistry; he adopts McLaughlin's distinction between resultant and configurational but he formulates it in terms of Hamiltonians, rather than forces. Using the quantum chemistry of the molecule, Hendry aims to show that there is downward causation in chemistry by showing that there are "configurational Hamiltonians" governing the behaviour of molecules.

Hendry asserts that if the behaviour of some systems is governed by configurational (non-resultant) Hamiltonians, then the behaviour of those composite systems is not determined by the more general laws governing their constituents. He argues that to the extent that the behaviour of any subsystem is affected by the supersystems in which it participates, the emergent behaviour of complex systems must be viewed as determining, but not being fully determined by, the behaviour of their constituent parts. This, Hendry contends, is the case in the physical chemistry of the molecule, where the motions of the atoms are determined by the overall structure of the molecule.

Hendry uses the concrete example of a CO₂ molecule. The parts of this molecule can be seen as quantum mechanical harmonic oscillators and rigid rotators. However, this is possible only after we assume a certain structure for the whole molecule. Hendry points out that we use quantum mechanics to explain the motions of parts of the molecule within the context of a given structure for the molecule as a whole (in this case, a linear structure). The problem is that rather than deriving this structure using resultant Hamiltonians, we put it "by hand"—we assume "configurational Hamiltonians". The fact that the motion of the parts of

molecule is determined by the overall structure is, according to Hendry, an example of downward causation.

Is the chemical emergence that Hendry's arguments support of a strong kind? If the molecular Hamiltonians are truly configurational and thus fundamental (i.e., not resultant), then the kind of emergence that Hendry's arguments support is strong. If, however, they are resultant, then Hendry's arguments support only weak emergence. The advocate of weak emergence may agree that the molecule as a whole constrains (determines) the motion of its parts. But she may argue that its ability to do so comes from the intrinsic and relational properties of the parts themselves (from the Coulomb attractive and repulsive forces between the parts and various other factors such as the Pauli principle, relativistic effects and even gravity). On this view, the use of configurational Hamiltonians is justified for pragmatic reasons (resultant Hamiltonians are just too hard to compute) or epistemic reasons (having to do with their explanatory role), but from an ontological perspective these Hamiltonians are ultimately resultant, albeit often unobtainable in practice. Nonetheless, Hendry's own view seems to be that the molecular Hamiltonians are not resultant, so he seems to regard chemistry as strongly emergent.

Hendry claims that his revision of traditional emergentism is at odds with the causal completeness (or causal closure) of physics—the thesis that “all physical events are determined (or have their chances determined) entirely by prior physical events according to physical laws” (Papineau 1990, p. 67). If chemistry truly denies the causal completeness of physics then it would seem that this constitutes evidence for a strong notion of emergence; presumably, the existence of non-physical but causally efficient properties (such as *sui generis* chemical properties) guarantees that what's true about them cannot be derived from the truths of microphysics. If one thinks that the causal closure of physics is grounded in the conservation of energy, it is not entirely clear how a strong version of emergence that denies it may respect this venerable principle of science.

Another recent approach to emergence in chemistry is due to Paul Humphreys (1996; 1997a; 1997b). Humphreys' account is original because it denies that the relationship between higher-level emergent properties and lower level properties is supervenience (1997a). Instead, it links emergence with the existence of a fusion operation that operates on *i*-level properties and outputs *i*+1-level properties, which have novel causal powers.

Humphreys' fusion process is formally represented as follows. Let $P_m^i(x_r^i)_{t_1}$ represent an *i*-level entity, x_r , instantiating an *i*-level property, P_m , at time t_1 . $P_n^i(x_s^i)_{t_1}$ will denote another *i*-level entity, x_s , instantiating

another i -level property, P_n , at time t_1 . Humphreys introduces the *fusion operation* symbolized by $[*]$, which takes as arguments the two property instances $P_m^i(x_r^i)t_1$ and $P_n^i(x_s^i)t_1$ and fuses them: $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$. The fusion operation is an i -level operation, i.e., an operation of the same level as its arguments. The result of the fusion operation is the fused property $[P_m^i * P_n^i](x_r^i * x_s^i)t_2$ at the $i+1$ -level, which can also be written as $[P_m^{i+1} * P_n^{i+1}](x_r^{i+1} * x_s^{i+1})t_2$. This property is what is emergent on Humphreys' account. The fused property is a unified whole in the sense that its causal effects cannot be represented in terms of the separate causal effects of the original property instances.

According to Humphreys, the non-separable states of quantum mechanics are examples of fusion emergence. A composite non-separable quantum system is holistic, in that the joint system possesses a state while the components taken individually do not. Given that quantum entanglement has a role in chemical bonding (via the Pauli Exclusion Principle), one would be tempted to claim that molecules are an example of fusion emergence.⁵

Humphreys' account of emergence was motivated by the desire to avoid the threats of the exclusion argument for reductionism, which states that higher-level emergent properties are excluded from affecting lower-level properties, since all the causal work is done by the latter (see Kim 1992; 1999; 2006). Humphreys argues that at the time when the fused property instance $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$ comes into existence, the original property instances $P_m^i(x_r^i)t_1$ and $P_n^i(x_s^i)t_1$ cease to exist. Therefore, it is *a fortiori* the case that they cannot compete as causes with the emergent property instance. On Humphreys account, emergents don't coexist with their bases, and this feature prevents the exclusion argument to get off the ground.

Humphreys explicitly suggests that his version of emergence challenges the assumption that the physical domain is causally closed (Humphreys 1997b, p. 3). The causal closure thesis asserts that the ultimate causes of all physical effects are themselves physical and is often taken to be

⁵ See Humphrey's conference talk titled "A defence of ontological emergence" which was presented at the International School on Complexity 9: Emergence in the Physical and Biological Worlds, Ettore Majorana Foundation, Sicily, in 2008. Since Humphreys has not turned this conference paper into a publication (yet), it is uncertain whether he is still committed to the view that molecules exemplify fusion emergence.

synonymous with the completeness thesis. Just as Hendry's emergentism, Humphreys' fusion emergence seems to be of a strong kind. Given that on Humphreys' account (some of) the properties of the parts are used up in the process of the formation of the whole, it would seem that a (synchronous) derivation of the properties of the whole from the properties of the parts is precluded in principle; this would further support the idea that fusion emergence is strong (synchronous) emergence.⁶

A number of contemporary authors have recently proposed concepts of emergence that are applicable to phenomena studied by science in general. Although the examples that these authors refer to come from specific domains (the theory of cellular automata, physics, etc) these concepts of emergence are applicable to a host of phenomena, including those in the purview of chemistry.

Mark Bedau (2008) thinks that there is not much room for strong emergence in contemporary science, and even if such strongly emergent phenomena existed, they could at best play a primitive role and thus they will be scientifically irrelevant. Bedau defends a version of emergence that he even refers to as "weak emergence". Weak emergence is compatible with the generality of microphysics:

Macro entities and their states are wholly constituted by the states and locations of their constituent micro entities, so the causal dynamics involving macro objects is wholly determined by the underlying micro dynamics. (Bedau 2008, p. 161).

But Bedau also recognizes that the global properties of a macro system may influence the behaviour at the micro-level. This is a sort of downward causation; however, the kind of downward causation is not the same as the fundamental kind of downward causation that is associated with strong emergence. The properties of the macro system (including the causal properties) are a consequence of the properties of the micro systems that compose it, but the derivation is usually hard to obtain. The hallmark of Bedau's weak emergence is that to obtain such a derivation there is no theoretical shortcut: one must resort to simulation. Bedau claims that causal processes in nature are caused by the iteration and aggregation of

⁶ This leaves open the possibility that what counts as strong emergence from the synchronous perspective would qualify as weak emergence if a diachronic notion of derivability is favoured. Besides these temporal aspects, the issue of whether Humphreys' fusion emergence is strong or weak is further complicated by various factors such as the nature of the fusion process and the potential differences between completeness and causal closure. This is not the place to address all these complications.

micro causal interactions. The only way to predict the macro properties of weakly emergent systems is to follow the same steps of iteration and aggregation that Nature follows, with the help of powerful computers.

Bedau's examples of weak emergence come primarily from the theory of cellular automata. For example, being a glider gun is a weakly emergent property in the Game of Life—a glider gun is a macro-level property, which is realized by a variety of micro-level configurations of cells. Thus, Bedau's emergence is compatible with a weak notion of reductionism—*token* reductionism, which claims that all property instances are lower level property instances; but insofar it is committed to the idea that the same macro property can be instantiated by a variety of different micro properties (see the multiple realizability of the glider gun example), Bedau's emergence is incompatible with *type* reductionism—the idea that all properties are lower level properties. According to Bedau, explanations that contain emergents (macro explanations) are autonomous in relation to micro explanations—they are overarching explanations that unify an otherwise heterogeneous collection of micro instances.

Concepts of emergence that emphasize context sensitivity, nonlinearity, feedback loops, and the importance of organization between the parts of compositionally complex systems have been presented by William Wimsatt (2000; 2008) and Sandra Mitchell (2010). These accounts of emergence are not intended to apply to chemistry in particular and they seem to be compatible even with a strong notion of reduction (type reductionism). This is why those inclined to see reductionism (or at least a strong variant thereof) and emergence as mutually exclusive would not readily embrace these accounts as emergentist. Indeed, what these accounts call "emergence" would actually count as "resultance" in the eyes of those who hold more conservative views about emergence.⁷

An emergentist account intended to apply to specifically to chemistry has been offered by Luisi (2002). By the term emergence Luisi understands the onset of novel properties that arise when a certain level of structural complexity is formed from components of lower complexity. Luisi emphasizes that molecular sciences, and chemistry in particular, are actually the disciplines in which the notion of emergence has the most obvious applicability. Luisi offers the following examples of emergent properties in chemistry: the aromaticity of a benzene molecule, which is not present in the atoms that form the molecule; the properties of water and of all other molecules, which are not present in the atomic components;

⁷ For a discussion of the distinction between emergence and resultance in the context of British emergentism, see McLaughlin (2008).

and the oxygen-binding properties of complex chemical structures like hemoglobin or myoglobin which are not present in the single aminoacids.

Luisi considers the following two questions. Can the properties of molecules be explained *a posteriori* from the properties of the components? Can they be foreseen *a priori*? Luisi argues that there are no reasons to think that the liquid properties of water, the aromaticity of benzene, or the folding of myoglobin, cannot be in principle explained or even foreseen on the basis of the properties of the components. Thus, Luisi seems to be entirely committed to token reductionism. He even goes as far as claiming that the hypothesis that the emergent properties of molecules cannot be explained as a matter of principle on the basis of the components is tantamount to assuming a force of some non-defined nature (Luisi 2002, p. 193).⁸ But he points out that in practice, emergent properties are almost impossible to predict. This is especially true for large molecules like myoglobin, in the case of which the 20 different amino acids and a chain length of 153 amino acid residues, gives rise to 20^{153} possible theoretical chains, myoglobin being one of those.

According to Luisi, chemistry offers examples of downward causation, understood as the influence of the relatedness of the parts on the behaviour of the parts themselves. One example that Luisi offers is that of benzene: when a benzene molecule is created, the orbitals of carbon atoms and those of hydrogen are changed; the molecule as a whole affects the properties of its constituents. Of course, it is true that the molecule of benzene could not have emerged if its components did not have the right properties (Luisi does not deny upward causation), but it is also true that once the molecule is formed it constraints the motion of its parts. For Luisi, downward causation is the consequence of upward causation, and once the two exist, they take place simultaneously in a sort of “cyclic” causality. But the kind of downward causation that Luisi endorses differs significantly from the kind of downward causation that the British emergentists talked about; it does not assume any special forces at work other than the normal laws of physics.

Luisi’s account of emergence resembles very much Bedau’s weak emergence, especially when one compares the two authors’ views about predictability and downward causation.

Another concept of emergence has been offered by Robert Batterman (2002; 2010). Although Batterman’s examples of emergence are primarily

⁸ It is plausible to think of this force of a non-defined nature that Luisi talks about as a “configurational force” in McLaughlin’s terms.

from physics, his view of emergence has the potential of applying to chemistry as well, and for this reason it is worth mentioning.⁹

Batterman distinguishes between two senses of reduction. One may talk of the reduction of one theory to another in the philosopher's sense (e.g., Nagelian reduction, where the laws of a coarse grained theory are derived from the laws of another, fine-grained, theory); or one may talk of reduction in the physicist's sense (the fine grained theory reduces to the coarse grained theory in the limit of some parameter having a certain value). For example, relativistic mechanics reduces to classical mechanics in the limit in which $(v/c)^2 \rightarrow 0$. Now, the limiting relations between theories may be *regular* (when the "limiting behaviour" as the parameter tends to a certain value resembles the "behaviour in the limit", where the parameter has that value), or they may be *singular* (when the behaviour in the limit differs markedly from the limiting behaviour). Many pairs of theories are related by singular limiting behaviour: quantum and classical mechanics, the wave and ray optics, statistical mechanics and thermodynamics.

For Batterman, the singular nature of the limiting relations between pairs of theories is indicative of emergence: the behaviour of the system as certain parameter approaches a certain value is different from the behaviour of the system when that value is reached. When the limiting relations are singular we can expect novel phenomena in the asymptotic regime between the two theories. Often, such in the case of thermodynamics and statistical mechanics, the coarser (higher level) theory can be derived (reduced in the philosopher's sense) from the fine grained (lower level) theory only if one makes the assumption that when a certain parameter (viz. the number of particles, N) approaches infinity. But real systems are always finite, and a strict derivation obtains only in the thermodynamic limit. As a result, one may speak of the phenomena of thermodynamics as emerging from statistical mechanics. Qualitative changes in the states of matter known as phase transitions (e.g., freezing and boiling water, the transition from the ferromagnetic phase to the paramagnetic phase) are also considered emergent since it proves very difficult (if not impossible) to reduce them to the underlying microphysics if we do not appeal to infinite idealizations.

⁹ In fact, if one regards thermodynamics and statistical mechanics as disciplines that equally fall within the purview of chemistry (as many chemistry textbooks do), Batterman's notion of emergence is applicable to at least this chemical example.

Batterman's approach pays close attention to mathematical procedures such as renormalization—a mathematical technique for characterizing how the structure of interactions varies with the scale considered. Renormalization reveals how theories at different levels are related, but such relation is not reduction: it turns out that the phenomena studied by the higher-level theory are decoupled from those at the lower level.

For Batterman, emergence is also associated with universality or multiple realizability (systems very different at the micro-level exhibiting identical macro-level behaviour). Multiple realizability shows that lower-level explanations cannot adequately account for the convergence of the behaviour of varied systems, and higher-level level explanations that ignore the micro-level details are required. In contrast with the classical notions of emergence, Batterman's notion of emergence does not subscribe to the downward causation thesis or to the idea that mereological part/whole relations play a crucial role in emergence.

There is another concept of emergence that applies to chemistry, but so far both chemists and philosophers of chemistry have not acknowledged it—I'll label it "functional emergence". Functional emergence refers to the idea that many chemical properties are defined not by a shared microphysical ingredient, but functionally, by a common behaviour. Take, for example, the property of being an acid.¹⁰ The property of being an acid is defined functionally, by pointing to a common behaviour of these substances in chemical reactions (the ability to donate a proton, on the Brønsted-Lowry theory) rather than to a shared microphysical ingredient (a hydrogen atom, for example).

Functional emergence is committed to the generality of microphysics: e.g. every acidic molecule is a complex microphysical system of interacting electrons, protons and neutrons, all obeying the laws of physics (token reductionism is respected). However, functional emergence agrees that it would be mistake to conclude from here that chemical properties are microphysical properties in disguise.¹¹ Similarly, it rejects the idea that if all events are governed by physical laws, then all laws must be physical. According to functional emergence, there are genuine chemical properties and laws, which are type-irreducible to the properties and laws of microphysics. The reason for this is multiple realizability: one and the same chemical property (e.g., acidity) is realized by a variety of

¹⁰ Many other examples of chemical functional properties can be given: being a base, an oxidant, a reductant, a metal, or being a piezoelectric.

¹¹ A chemical property is a physical property in disguise if the chemical property is identical with a very complex physical property but this identity relation is not obvious.

microphysical lower level properties (systems of electrons, protons and neutrons), and thus it cannot be identified with any particular microphysical constitutive property. As a result, the laws in which functional chemical properties occur will not be derivable from the laws of microphysics simply because the latter lack the requisite terms. Since derivability seems to be impossible in principle, functional emergence seems to qualify partially as strong emergence. I say partially because only the chemical laws that contain terms denoting functional properties cannot be derived, but particular chemical events may still be predictable from the underlying physics. However, unlike other varieties of strong emergence, functional emergence does not go as far as to deny the causal closure of physics.

Conclusion

Developing accounts of emergence in chemistry is important because emergence typically offers a way of reconciling the failure of reduction with the commitment to the generality of microphysics. In addition, emergence seems a promising way to secure the ontological autonomy of chemistry. If a theory of chemical emergence can demonstrate that chemical properties are not just complicated microphysical properties in disguise, then chemistry is autonomous from microphysics not only from a historical, epistemic or pragmatic point of view, which is never contested, but also from an ontological one, which is more problematic.

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