Philosophy of Science and Philosophy of Chemistry

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Abstract: In this paper I assess the relation between philosophy of chemistry and (general) philosophy of science, focusing on those themes in the philosophy of chemistry that may bring about major revisions or extensions of current philosophy of science. Three themes can claim to make a unique contribution to philosophy of science: first, the variety of materials in the (natural and artificial) world; second, extending the world by making *new* stuff; and, third, specific features of the relations between chemistry and physics.

Keywords: *philosophy of science, philosophy of chemistry, interdiscourse relations, making stuff, variety of substances.*

1. Introduction

Chemistry is unique and distinguishes itself from all other sciences, with respect to three broad issues:

- A (variety of) stuff perspective, requiring conceptual analysis of the notion of stuff or material (Sections 4 and 5).
- A *making* stuff perspective: the transformation of stuff by chemical reaction or phase transition (Section 6).
- The pivotal role of the relations between chemistry and physics in connection with the question how everything fits together (Section 7).

All themes in the philosophy of chemistry can be classified in one of these three clusters or make contributions to general philosophy of science that, *as yet*, are not particularly different from similar contributions from other sciences (Section 3). I do not exclude the possibility of there being more than three clusters of philosophical issues *unique* to philosophy of chemistry, but I am not aware of any as yet. Moreover, highlighting the issues discussed in Sections 5-7 does not mean that issues reviewed in Section 3 are less important in revising the philosophy of science. Section 2 briefly summarizes causes of the neglect of chemistry in the philosophy of the sciences (plural!).

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Three categories are needed to order materials in the natural world or produced in the laboratory or chemical industry (Section 4):[1] (thermodynamic) phases, (macroscopic) chemical substances, (molecular-scale) chemical species.

If chemistry had been the 'first science' in the philosophy of science, that would primarily have meant the addition of the clusters reviewed in Sections 5 and 6 as well as rather different research programs for the existing theme of 'how everything fits into one world' (Section 7). Some of the issues reviewed in Sections 5-7 are important additions to philosophy of science; some issues substantially change existing themes in the philosophy of science. An important example of the latter is the notion of natural kind.

The issues here presented as philosophically importantly different or unique as to chemistry, apply to experimental physics and/or materials science to a considerable extent as well. Traditionally, physical chemistry (including chemical thermodynamics, quantum chemistry, phase theory, colloid science, electrochemistry, surface chemistry) is part of chemistry.[2] In addition, in the broad view of philosophy of chemistry advocated in this paper, most of 'materials science' is included (characterization and production of composite materials, polymers, metal alloys, ceramics, biomaterials, semiconductors), as well as parts of solid state physics, chemical engineering science, pharmaceutical technology, nanotechnology, molecular biology, biomedical sciences, earth sciences (geology, mineralogy, petrology), and environmental sciences.[3]

This paper is primarily based on recent post-2000 publications in philosophy of chemistry. For reviews of pre-2000 publications see Schummer 2006a and van Brakel 2000.[4] History of chemistry and chemical education is not included in this paper. Some views or relevant publications will only be mentioned in passing. There is no space for critically discussing all of them.

2. The neglect of the philosophy of chemistry

Until about 1960, English-language dominated philosophy of science mainly consisted of philosophy of physics. In the eighteen parts of the *Foundations of the Unity of Science: Toward an International Encyclopedia of Unified Science*, published between 1938 and 1970, the only references to chemistry can be found in Thomas Kuhn's *The Structure of Scientific Revolutions* (1962) and, significantly, a few pages on chemical bonding in Philipp Frank's contribution on the foundation of physics (1946).[5]

There is extensive literature discussing the possible causes of the neglect of chemistry in the philosophy of science and there may be some truth in every suggestion made. I suggest the major long-term cause is the highly influential pronouncements on the status of chemistry by first Kant and more recently Dirac (van Brakel 2006, pp. 71-2).

Pre-1960 interest by philosophers of science was almost exclusively in *theoretical* science. Putting the emphasis slightly differently, physics and chemistry were lumped together as *exact* natural sciences with focus on studying its *logical* structure. This meant that the interest was in laws in the sense of mathematical equations stating relations between quantities and theories that were axiomatic, at least in principle. Mainstream philosophy of science simply regarded chemistry as part of physics and an unimportant part at that, the general impression being that with the quantum mechanical interpretation of the chemical bond, chemistry had been reduced to physics. If there might have been some philosophy of chemistry in the pre-quantum era, with the advent of quantum mechanics, it became irrelevant at one fell swoop. This applied in particular to the German *Naturphilosophen* and the British emergentists.

Chemical examples might be used in the philosophy of science or even in other parts of philosophy.[6] But usually such examples had little to do with what might be considered typically chemical. Still, in the 1960s a few isolated publications focusing more specifically on chemistry appeared. Most of them can be seen as reporting falsifications of universal features of 'the' method of science. For example, it was reported that received views on theory and explanation and their relation to experimental data were not confirmed by chemical practice. However, neither the republication in 1962 of Paneth's 1931 article, nor the contribution of Caldin (1961), both in the *British Journal for the Philosophy of Science*, received any lasting follow up.

Authors defending the autonomy of chemistry and its philosophy, might still start by saying philosophy of science is taught around the world from a positivistic perspective (Bensaude-Vincent & Simon 2008, p. 4). However, since the 1970s this is not true anymore. At present philosophy of science is fragmented in many approaches, without any dominant grand narrative. Different strands emerged in the philosophy of science and there has been some impact from other traditions (such as phenomenology and French philosophy of science). Interest arose in historical case studies to provide arguments for and against the rationality of scientific progress or development, both within philosophy of science 'proper' and in the sociology (or anthropology) of science. As a consequence, the number of papers on the history of chemistry that included some philosophical considerations increased considerably.

Interest in the experimental side of natural science developed, as well as a reaction against the bias within philosophy of science towards (formal) theory. This development also favored the appearance of more references to chemists. In Hacking's *Representing and Intervening* (1983) there are discussions of Boyle, Dalton, Davy, and Lavoisier, as well as references to Berzelius, Brønsted, Kekulé, Lewis, Pasteur, William Prout, and von Liebig. In Latour's *Science in Action* (1987) there are more references to Crick, Mendeleev, and Pasteur than to Einstein, Newton, and Copernicus.

These changes in mainstream philosophy of science started to have some impact on restoring the balance between chemistry and physics in philosophical discourse. However the more influential contributions focused on physical case studies. Moreover, many chemical case studies are not concerned with what might be specific to chemistry. Usually they 'test' positions in general philosophy of science ('models' of Popper, Lakatos, Laudan, Hacking, Latour, *etc.*).

It was only in the 1990s, due to a variety of contingent factors (van Brakel 2012a, pp. 40-1), that philosophy of chemistry emerged, first in several European countries, leading to a truly international endeavor in the recent decade. In the late 1990s, six conference proceedings appeared, dedicated to philosophy of chemistry,[7] and from 2000 onwards, there were not only two journals catering for the philosophy of chemistry, but an increasing number of philosophy of chemistry papers appeared in mainstream philosophy journals.

However, the days of neglect are not over, as the following typical examples show. In the highly acclaimed *Philosophy of Science: The Central Issues* (Curd & Cover 1998, second edition 2012), a selection of about 50 articles representing the philosophy of science, there is not a single article from the philosophy of chemistry.[8] Chemistry is mentioned about 50 times in the context of a brief reference to the 'chemical revolution'.[9] Otherwise the word 'chemistry' often occurs in the phrase 'physics and chemistry', when talking about science in general, but there is no serious reference to chemistry of the twentieth century. Typically, when the author of one article writes: "the only 'genuine' theories will be found in physics and chemistry" (Resnik 1998, p. 1182), the editors, in their discussion of this article, change the author's opinion to "theories are confined to physics and *perhaps* chemistry" (Curd & Cover 1998, p. 1266, emphasis added).

Also in the context of history and philosophy of science, physics and chemistry are often mentioned in one breath. But the overall terminology of the discourse shows no signs of chemistry being a science in its own right. For example, Galison, in a 2008 article in the journal *Isis* proposing "ten problems in history and philosophy of science", often mentions chemistry (and biology, and earth sciences, and physics), but when he raises the question, "what counts as purity in mathematics, physics, chemistry, biology?", the author is not thinking of pure substances in chemistry (but of the distinction between pure and 'impure' science).[10]

3. Contributions to general philosophy of science

In this Section I list a number of themes in general philosophy of science to which philosophy of chemistry can make important contributions changing the face of philosophy of science. Some of the themes reviewed here may still develop into *unique* contributions of philosophy of chemistry to philosophy of science.

There is a considerable range of concepts in chemistry that warrant conceptual analysis, as 'rough ground' for the philosophy of chemistry (and chemical education).[11] In addition to laying the foundations of chemistry, these concepts warrant analysis because they bear on the main themes discussed in subsequent Sections. However, the method of conceptual analysis in the philosophy of chemistry is not much different from conceptual analysis with respect to other discourses.[12]

It has been remarked that chemistry has no *procedure* for doing science (*e.g.* falsification); the connecting thread is a continuing story or making up stories (Hoffmann 2007). This suggestion has also been made with respect to other sciences. A more specific feature of chemistry is that its development does not merely consists in new explanations, theories, and the refinement of methodology, but also in making new materials (see Section 7).

Philosophy of chemistry offers several interesting case studies for the realism debate, for example the question whether orbitals 'exist' (Labarca & Lombardi 2010, Mulder 2010).[13] The latter issue is also relevant for the notion of observation (Mulder 2011, Ogilvi 2011). In general, chemistry will suggest a more realistic metaphysics than other sciences, because it is making things. However, in the philosophy of chemistry no 'new' notions of realism have been proposed, which is not surprising as there are already about twenty varieties in general philosophy of science (not counting realisms in other parts of philosophy).[14]

Philosophy of chemistry has shown that simple forms of essentialist realism are falsified by chemistry. Soon after the influential publications by Kripke and Putnam, their defense of essences discovered by science being *a posteriori* and necessary was criticized, because of overlooking the rough ground of chemical knowledge (Mellor 1977, van Brakel 1986, 1990).[15] Later publications added more detail, in particular concerning features of water, but there has been a lot of repetition as well.[16]

Chemistry may provide important case studies undermining the distinction of primary and secondary qualities (Bhushan & Rosenfeld 2000, p. 8; Earley 2003b). Different techniques will only determine the same shape (of a molecule) if they operate at the same time scale (Ramsey 2000).[17] The shape of molecules does not neatly fall in either the primary or secondary category.

Repeatability and reproducibility in experimental chemistry is somewhat different from other experimental sciences (Plesch 1999), but does not raise particularly new issues. The issue of ontological commitments in the design of instruments (for example as used in analytic chemistry) and properties being highly responsive to techniques of instrumentation (Rothbart 2000) is equally relevant to other experimental sciences such as biology and psychology.

There is no consensus as to what qualifies as a *chemical* law, emphasizing either that there are few (laws of definite, multiple, and reciprocal proportions) or many (all chemical equations). The periodic system of elements has been referred to as a central law, model, or theory of chemistry, but it may also be considered a classification that organizes a vast amount of information and is capable of making testable predictions (Scerri 2012, p. 329f). In the latter understanding it forms part of the semiotics of chemical space (see Section 6). Perhaps in view of the cachet of philosophy of chemistry, it might be wiser to present the periodic system as a major fundamental law of nature that lies at the basis of the unlimited variety of chemical substances and their transformations.[18] More relevant to our theme is that it is a philosophically interesting law because it is primarily a case of non-mathematical and non-linguistic representation.[19]

It has been argued with some force that whatever chemical laws there might be, they will always have exceptions and are only valid in limited circumstances.[20] Water boils at 100°C, but not always (Chang 2007, van Brakel 1986). Hence, chemical laws are not universal in some strict sense. Mainstream philosophy of science and philosophy of mind assume that (theoretical) physics is the only science concerned with strict laws; all other sciences are special sciences, where we find only *ceteris paribus* laws, as in chemistry. However, this traditional view, almost universally shared among philosophers and other people, has been thoroughly criticized by Cartwright (1999), who has defended the view that *all* (theoretical) laws are *ceteris paribus*. She has argued that theoretical (fundamental) laws apply to models, which, strictly speaking do not exist in the real world. Models deliberately construct falsifications of 'reality' so that theory can deal with them. Philosophy of chemistry can provide ample evidence to support this view (van Brakel 2004, pp. 27-30). Moreover, contrary to Cartwright's view, phenomenological laws are *ceteris paribus* as well (van Brakel 2012c, p. 543). Phenomenological equations apply to phenomenological models, which deliberately construct falsifications of 'reality', hoping that nevertheless the model will allow sufficiently adequate predictions of some piece of reality. At best the phenomenological models apply to their material realizations in highly regimented laboratory conditions.[21] If chemistry would have been the main focus in philosophy of science, the chapter on scientific laws would have been very different, but this can also be said of other 'special' sciences.

Approximations (in quantum chemistry, with respect to pure substances, in chemical engineering science) are ubiquitous, but not unique to chemistry. As in other sciences there are many different kinds of models employed in chemistry.[22] Most uses are not significantly different from the use of models in other sciences. There are two possible exceptions. First, there is the conceptual notion of pure substances as a model of chemical substances and reference point for all materials (Section 5). Second, there is the created reality in the laboratory or chemical industry as a model of the messy reality out-there, providing 'ideal' boundary conditions (contexts) for chemical reactions and down-stream processing (isolation and purification of products).[23] Models in chemistry and chemical engineering fit, in particular, bits of the world inside laboratories or the chemical industry, where the idealized boundary conditions can be approximated.

Mereology can be applied to many sciences (Calosi & Graziani 2014). Also chemistry does not fit easily in classical mereology (which the simplified notion of atoms in molecules might suggest) and many modifications and extensions have already been proposed. Philosophers of chemistry may make new contributions to mereology as a theme in mathematical logic. Issues raised as requiring extensions or revisions of classical mereology include:[24]

- Individuals enter combinations of interesting sorts. They no longer are the very same individuals that existed prior to the composition.[25]
- Quantities of matter cannot always be considered a collection of molecules or atoms. Temporal and modal parameters have to be taken into account.
- Different mereological partitionings of a molecule are possible. This may lead to different conceptions of 'atom in a molecule'.
- Open-system dynamic coherences are defined by their capacities to act on their surroundings, which is difficult to fit in.[26]
- Parts and wholes differ depending on the levels of calculation or the apparatus being used.

Several authors have pointed out the special role of visual representation (diagrammatic representation, structural formulae) in chemistry.[27] Sophisticated representational schemes may be paradigmatically explanatory: "without the diagrammatic and graphical techniques, the mathematical results would have remained largely sterile" (Woody 2012, p. 457). Because structural formulae are not truth bearers, they cannot function as premises in a DN-scheme (Goodwin 2009b).[28] Formulae are both descriptive names and models. They describe the composition, connectivity, and spatial arrangement. However, figures, pictures, diagrams are ubiquitous in many sciences. The use of diagrammatic non-linguistic representation in chemistry, raises the old question of the necessity of models for explanation (Hesse 1966).

Already in the 1960s it was reported that chemical explanation does not fit Hempel's deductive-nomological model of explanation (Churchman & Buchanan 1969). However, notwithstanding a whole volume on chemical explanation (Earley 2003a), it seems that explanation in chemistry only changes the relative plausibility of different existing theories of explanation, not that chemical explanation as such is unique. Different authors in philosophy of chemistry have advocated various causal theories of explanation,[29] have followed Bas van Fraassen's (1980) pragmatic stance with respect to explanation, or even used Hempel's deductive-nomological scheme (Hettema 2012a). Cartwright's elaborations of the notion of capacity might be relevant as well to explanation in chemistry. For the moment the jury is still out on the issue of chemical explanation; "it is too early for any consensus to have emerged" (Akeroyd 2008, p. 39). "None of the standard accounts of explanation fits this case neatly, and yet all of them seem somehow relevant" (Woody 2012, p. 462). The latter may well apply to other cases and disciplines.

Traditional philosophy of science regards theoretical reasoning, based on the example of Euclidian geometry, as the hallmark of a mature science.[30] There is, however, a parallel tradition of practical reasoning based on specific cases that goes back to Aristotle. Chemistry is less concerned with 'pure' theoretical knowledge than with practical control and change of poetic practices, *i.e.* practices that aim at the production of material goods (Janich 1994). Schummer (1997b) argued that chemistry challenges the distinction between natural science and technology.[31] Bensaude-Vincent (2009, p. 166) has suggested that chemistry is not a natural science, but "a cornucopia of material technologies". But one should not too quickly associate chemistry with technology. Although for both action is central, most of technology is concerned with the design and production of 'things' composed of parts made of existing materials which have already been given a specific form. In contrast, chemical and material engineering, if considered technology, are concerned with the production of (bulk) materials out of other stuff. In the case of chemistry (or chemical technology) the distinction between artificial and natural kinds is undermined (see Section 6), which is not typical for most technology. One can argue that chemical knowledge is at the same time epistemic and theoretical, even transcendental, as well as knowledge directly useful for making stuff. However, the issue of science, technoscience, technology, and techniques can be addressed with respect to many sciences (including physics and social sciences).[32]

Many developments in nanotechnoscience can be seen as an extension of interface/surface chemistry, which involves the study of thin molecular layers adjacent to interfaces and therefore may be considered interphases. Molecular nanotechnology, *i.e.*, producing molecular devices, is not fundamentally different from supramolecular chemistry that emerged earlier, without being called nanotechnology (Schummer 2006b). Surface chemists involved in nanotechnology are basically doing the same thing as what they were doing half a century ago. More important, but not an issue for the philosophy of chemistry, is the undermining of the distinction between technology and the (natural) process of biological evolution and 'life'.

Chemical research, whether in academia or in industry, whether pure or applied, has ethically relevant aspects. But these issues are not fundamentally different from the general theme of science and ethics/society. Questions such as what to research and what to make (and how) have often neglected ethical or political aspects, but this is so for all science in one way or another. Concern about safety or sustainable development is relevant to many sciences. It has been suggested that predicting the properties of new chemical substances is radically incomplete and therefore raises specific ethical questions in connection with their consequential properties and effects (Schummer 2001, pp. 110-1; 2010, p. 180). However, description, prediction and consequences of adding artifacts to the world are always incomplete. Radical incompleteness is not more incomplete than incompleteness. The Problem of Complete Description (called the frame problem in Artificial Intelligence) applies across the board and is a necessary feature of all knowledge and practices (van Brakel 1992b).

By comparing chemistry to art, chemists have made claims concerning the aesthetic value, even beauty, of some of their products. Here chemistry makes a novel contribution to aesthetics,[33] but does not require major changes in aesthetic and/or semiotic discourse.

4. Three basic categories: Phases, substances, species

This Section is a terminological intermezzo in preparation of Sections 5- 7.[34]

Chemistry can be defined as the science of the characteristics of (macroscopic) materials or phases (including phase transitions) and their containing (molecular-scale) species, as well as the (planned) interaction of these materials with other materials (synthesis, chemical transformations, separation methods). Three ontological categories are needed to bring some order to the variety of materials: the notion of phase, the notion of (pure) chemical substance, and the notion of chemical species, which are closely intertwined, but not reducible to one another.[35] I am not claiming that this is the only 'true' way of ordering the ontology of chemistry. Other proposals are welcome.

Materials can be divided into (heterogeneous) conglomerates (of phases) and (homogeneous) phases.[36] A phase is a homogeneous body of continuous matter that is characterized by its chemical composition and thermodynamic state without regard to its size or shape or any atomistic assumption concerning constituting species (Gibbs 1931).[37] A phase consists of one or more substances and a substance may occur in more than one phase.[38] Apart from solid and liquid phases and the gas phase, there are many other kinds of phases, for example amorphous,[39] colloid, and superfluid phases; stable non-stoichiometric phases and metastable phases.[40] The notion of phase brings with it the phase rule and the notion of component (in the sense of the phase rule).[41] The latter notion is different from that of chemical substance and chemical species. The number of components and the number of substances in a quantity of matter is not always the same.

Prototypical pure substances occur in at least one solid phase, a liquid phase, and a gas phase and can also be defined/identified in terms of their one-component-phase diagram, triple point(s) 'connecting' the phases.[42] Many substances have a considerable number of different solid phases (in particular at high pressures and/or low temperatures). Binary phase diagrams may contain many intermediate compounds.[43] Substances can be divided into pure (stoichiometric) substances (compounds and simple substances), intermediate substances (including addition compounds), non-stoichiometric compounds,[44] and, perhaps separately,[45] one-phase only materials. The distinction between these subclasses of substances is rather fuzzy.

A pure substance can also be defined as a substance of which properties of two coexisting phases remain invariant during a phase transition, which takes place at a constant temperature (and pressure). If the phase transition is also reversible, it will be referred to as a *classical* phase transition.[46] If a homogeneous material does not meet the criterion of classical phase transition, it is a mixture of substances, called a solution. Solutions are phases containing more than one substance.[47] An impure substance is a solution. Hence the phrase '(chemical) substance' always refers to the ideal of a pure substance. Phases can be separated by mechanical methods. Solutions can be separated by thermodynamic methods, for example distillation.[48] Homogeneity is relative to accuracy and scale of observation. Hence, the border between solutions and conglomerates is fuzzy.

Operationally a (simple or compound) substance is pure if it is perfectly homogeneous after being subjected to successive modes of fractionating which are as different as possible and when attempts at further separation/purification produce no further change in properties. Later refinements may show that what was once thought to be a pure substance is, after all, not pure. The ideal pure substance would pass all types of ideal purification tests, *i.e.* tests with unlimited resolution. Separation and purification reduce the continuity of materials to a discrete ordering of pure substances, thus providing a frame of reference to locate substances and their transformations.[49] The chemist's models for pure substances rarely apply to the natural world.[50] Chemists make substances in the laboratory and put them in bottles, in order to further investigate them. Therefore Schummer suggests, "the material world is thus adjusted to the conceptual needs" (2010, p. 168). This feature may be extended to the chemical industry (van Brakel 2012c).

Homogeneous materials with the same chemical composition can be different substances (isomers, stereoisomers, enantiomers, polymers, tautomers).[51] The same substance may occur in more than one liquid or solid phase (polymorphs, allotropes). The number of substances is not always easy to determine, depending on the interpretation of phase diagrams and chemical species the system contains.

Perhaps we should limit the notion of substance to what can exist independently in containers or is (sufficiently) similar to species that can.[52] As to the latter, consider einsteiniumastatide, $EsAt_3$. Einsteinium and astanium are simple substances, but occur in such small quantities that producing macroscopic quantities of $EsAt_3$ is out of the question. Nobelium only exists in the form of a few atoms at a time. By extension we might consider cases like this 'theoretical' substances, even though they do not fit the operational definitions. Substances or species that exist in only one phase, easily decompose, only occur in solution, *etc.* can only be included by analogy.

Chemical substances defined operationally in terms of a sequence of purification/separation methods should be distinguished from chemical species (typically identified using spectroscopic techniques).[53] Chemical species are hypothetical constituents of substances or phases, such as molecules, ions, radicals, oligomolecular and supramolecular aggregates, atoms in ordered or disordered solid structures, held together by various types of interactions (ionic, covalent, metallic bonds; hydrogen bonding, ion pairing, metal-to-ligand binding, spin-spin interaction, van der Waals attractive forces, *etc.*).

Often a substance contains many species (in equilibrium). A material, phase, or substance has a (macroscopic) chemical composition and a (molecular) species composition. The range of species present depends on temperature, pressure, and other contextual variables. Philosophers often incorrectly identify a pure substance with one particular species. Water is *not* a collection of H_2O molecules.

Chemical (molecular) species that cannot be put into bottles, cannot be subjected to any reversible phase transition, occur only in solutions or other special environments,[54] only 'exist' in excited stages, or have an extremely short half-life, may have a full claim to being a chemical species, but may not claim to be (pure) substances. If the species only exist in equilibrium with other species 'inside' pure substances or solutions,[55] or figure only in reaction mechanisms and cannot be separated as independent substances, they can be accepted as (hypothetical) species, but not as substances. This includes radicals, reactive fragments, activated complexes, ligand-receptor complexes.

Although a tautomer may contain two species as different as ethyne C_2H_2 and benzene C_6H_6, under particular experimental conditions, the dynamic isomer may have a triple point and meet other criteria of being one substance and one component in the sense of the phase rule. Usually substances have a more independent existence in a way that many species have not, but also substances have a limited range of existence.

Enantiomers may form racemic mixtures and in solution may display rapid racemisation.[56] The two pure enantiomers have identical thermodynamic properties and most other properties, including phase behavior and reaction rates with achiral reagents, are identical. Because of the entropy of mixing, a racemate is more stable than either enantiomer. Differences between optical isomers arise in the presence of other chiral molecules or objects. Therefore, two enantiomers fit differently into the enzymes that drive biochemistry. Although enantiomers are thermodynamically identical, equally stable, and have the same spectra, one still would be inclined to say that they are two distinct species as well as two distinct substances (because some can be separated by hand, as Pasteur did).[57] Because optical isomers have no intrinsic difference in their shapes, they present a problem in the philosophy of space.[58]

$ArCl_2$ van der Waals complexes and $ArCl^+$ polyatomic ions may (or may not) meet the criteria of entity realism, but they cannot be put into bottles.[59] Also their identity conditions are evanescent. $ArCl_2$ has an estimated lifetime of 10^{-12} seconds, but may properly be considered to exist (Earley 1998). Such rare species are identified in solution using spectroscopic techniques, perhaps supported by *ab initio* calculations. There is a large range of 'fleeting species' (Berson 2008) in between some classical substance which can be put into bottles, being more or less pure (such as water or benzene) on the one hand, and the knowledge that in a certain space-time region certain amounts of particular atoms hover round and interact to a greater or lesser extent (*cf.* Vemulapalli 2008, p. 41).

There is no all-encompassing chemical species concept that can encompass their enormous variety, except for the very general notion of arrangement of sets of nuclei and electrons.[60] Hence a reductionist interpretation of materials in terms of something called 'molecule' (even if ions, *etc.* are included) is not possible and one has to fall back on the level of nuclei and electrons as underlying basis. Nevertheless, as Bishop (2010, p. 171) puts it: "Molecular structure is a necessary condition for chemistry."

Perhaps the 'imposed' terminological classification above can give an inkling of the complexities of (chemical) stuff. No sharp distinctions are possible. The old-fashioned idea of giving strict definitions in terms of necessary and sufficient conditions fails. The ordering of 'stuff' is better approached from the perspective of family resemblance concepts (having fuzzy borders and no 'essence').[61] This is further supported by the remaining Sections of this paper.

5. Chemical substance(s) – 'stuff'

Philosophical issues related to the notion of 'chemical substances' are a unique contribution to general philosophy of science and analytic metaphysics. These issues are significantly different from discussions concerning natural kinds or categories in connection with other sciences (*e.g.* fundamental particles in theoretical physics, species in biology, alleged natural kinds in brain and behavioral sciences). By focusing on 'stuff-kinds' instead of 'atoms', we will see that the stuff of the world cannot be neatly divided by (allegedly) 'cutting nature at its joints'.

The first issue is whether, ontologically speaking, the world consists fundamentally of one kind of matter or of a great variety of materials; *i.e.* the distinction between the ontology of matter in general and the ontology of particular kinds of matter (van Brakel 1991).[62] Explicit statements concerning this distinction, often in connection with statements concerning atomism and/or the autonomy of chemistry, can be found in the writings of numerous chemists and philosophers in the past few centuries. Bachelard argued for metachemistry ("the prodigious variety of the changes [*devenirs*] of matter"), in contrast to metaphysics (which focuses on one substance only).[63] In his later life Kant might have been developing a similar view. Already in the *Dantziger Physik* of 1785 he wrote:[64]

> Chemistry has raised itself to greater perfection in recent times; it also rightfully deserves the claim to the entire doctrine of nature: for only the fewest appearances of nature can be explained mathematically – only the smallest part of the occurrences of nature can be mathematically demonstrated. Thus, *e.g.*, it can, to be sure, be explained according to mathematical propositions when snow falls to the earth; but why vapors transform into drops or are able to dissolve – here mathematics yields no elucidation, but this must be explained from universal empirical laws of chemistry.

The consequences of the limits of *a priori* mathematical physics, of the rise of chemistry as a quantitative science, and of the need for a philosophical account of the variety of substances (which Kant started to see as a gap in his philosophy), Kant developed in his *Opus posthumum* (van Brakel 2006).

Individualistic or atomistic metaphysics was 'confirmed' by the final success of atomism around 1900.[65] But already for a long time, European natural and formal languages presupposed an ontology of individuals. The ontology of chemistry might suggest an alternative view: to see the world as a mass of various materials (various kinds of stuff), which are in constant change due to interaction with their environment (*i.e.* other stuff).[66] Properties and dispositions should not be ascribed to individuals but to a mass of stuff.[67] Perhaps the notion of affordances in the extended meaning of 'to make available possibilities', would suit the philosophy of chemistry better than the notion of individuals having (dispositional) properties.[68]

Stuff and individual are fundamentally different ontological *categories* (Schummer 1995, 2008; Lewowicz & Lombardi 2013). The history of Western philosophy is biased towards viewing the world as a collection of individuals. Individuals have primary qualities; substances have relational, extrinsic properties (depending irreducibly on context). All material properties are dynamic *relations*. An important difference to physics and standard conceptions of science is that substances can be placed in an experimental context independent of size, form, parts, or coordinates (Schummer 1998a, p. 132; *cf.* 2008).[69]

In passing it may be noted that it has been argued that philosophers in ancient China should be interpreted as tacitly believing that the world should be analyzed, not only in terms of parts and whole(s), but in addition (or even primarily) by dividing down (from the whole to the parts), instead of analyzing the world in terms of 'atomic' individuals and sets, *i.e.* building up.[70] The one-many 'entity' assumption is typical for the history of Western philosophy. Attributing a part-whole 'stuff' assumption to Mohist, Confucian, and Daoist thinking might give a better interpretation of their respective views concerning 'the world'. One of the consequences would be that the Chinese character *wu* 物, usually translated as 'object, thing', should be translated as 'stuff-kind'. The world (universe) consists of a myriad of stuff-kinds (*wanwu* 萬物), not of objects.

In addition to highlighting stuff-kinds, de-essentialization of the notion of chemical substance provides further support for de-reification. Although the precise meaning of 'non-stoichiometric compounds' (or berthollides) is contested,[71] the omnipresence of non-stoichiometric compositional formula in various parts of inorganic chemistry (including metallurgy, ceramics, soil science, *etc.*) cannot be doubted, for example the composition of illite, $K_{0.62}Si_{3.51}Al_{2.03}Mg_{0.19}Fe(III)_{0.29}O_{10}(OH)_2$ or reference to stable non-stoichiometric phases in the system $Sr_{1-x}Bi_{2+2x/3}Ta_2O_9$ (x=0-0.5).[72] These two examples might be reinterpreted as complex solutions. Iron oxide under the name of wüstite is less disputable, having a stoichiometry of something like $Fe_{0.86-0.94}O$ and definitely behaving as a one-component system.[73] Transition metal oxides are not the only examples of deviations from stoichiometry.[74] It may be a general feature of crystalline phases (Kosuge 1993).[75] However, what superficially looks like a case of non-stoichiometry, may be a case of stoichiometrically 'big numbers' as they appear in homologous series of intermediate compounds such as $Nb_5O_{2.49}$ (which is $Nb_{53}O_{132}$) and clathrates or complexes such as $Ar(H_2O)_{5.67}$.[76]

It has been argued that the distinction between non-stoichiometric compounds and solutions is one of convenience (Earley 2005). For example, in some situations titanium hydride is best considered a compound, in other situations a solution. Perhaps at low concentrations it may be considered a solution, whereas at higher concentrations, non-stoichiometric compound phases may form, all the way up to the 'true compound' TiH_2. How should we draw the boundary between solutions and non-stoichiometric compounds? Whatever the answer is, it is clear that pure stoichiometric substances fulfill an important role, but the range of 'perfect' materials is much broader, no matter whether they are called solutions or non-stoichiometric compounds. Quasi-homogeneous conglomerates (*e.g.* concrete) can also be 'perfect' materials.

Interest in non-stoichiometric compounds has been marginal in chemistry.[77] With rare exceptions, research on non-stoichiometric substances only occurred in the margin of materials sciences. František Wald was one of few chemists, who, around 1900, committed himself to develop a theory of chemical substances for the general case of non-stoichiometric substances, taking the notion of phase as fundamental.[78] This view is certainly not without justification.[79] Wald was right in stressing that stoichiometric substances are a special case, as the current increasing importance of so-called composites and the move from a pure-substance-discourse to a phase-discourse illustrates.[80] Many old and new composites do not claim to be (pure) substances. In designing multicomponent high-entropy alloys (such as $AlCoCrFeNiTi_x$), one may prefer the formation of solid solution phases, *i.e.* mixtures, instead of (stoichiometric) intermetallic compound phases, *i.e.* (allegedly) pure substances.[81] In fact, *all* substances are impure (*cf.* Bachelard) and sometimes the impurities make the relevant properties. Chemistry is an impure science (Bensaude-Vincent & Simon 2008). Traditional, modern, and hypermodern practices all aim at producing *both* pure and impure substances or mixtures, although there is a tendency for chemists to focus on pure substances or a couple of molecules,[82] leaving the real stuff, whether pure or not, to materials science.

Often perfect materials were produced before anything was known concerning their ontological status. For example, in the history of making hard steel, austenite, lederburite, and cementite were identified as different materials with rather different characteristic properties, long before 'theory' told us that lederburite is an eutectic mixture (solution) of the phases austenite (a saturated solid solution of the component C in the component Fe) and pure cementite (Fe_3C), a stoichiometric compound.

A strict distinction between stoichiometric and non-stoichiometric 'definite' compounds (or compounds with variable composition such as $TiO_{1.983-2.000}$), as well as that between solutions and non-stoichiometric compounds, should not be insisted upon. Because, in the end, '(chemical) substance' is a proto-scientific concept (not defined in science) and because identification (isolation, separation) depends on specific properties that are considered relevant and must be known, 'substance', no matter how defined in relation to solutions and non-stoichiometric compounds, will remain a pragmatic notion. Ambiguous situations may arise as to whether to count a sample as one, two, or three substances.[83] In such cases, substance identity is best correlated with its possible isolation, as distinct from components or 'phase rule substances' (identification via a phase diagram) and individuation of chemical species via interaction with electromagnetic radiation. Stimulated by the proliferation of more and more polymorphisms of well-known (simple) substances and intermediate compounds in binary systems, as well as the proliferation of new substances existing in one phase only or as metastable phases, there will be an increasing tendency to divide the material world into phases (of materials/species).

How to relate the categories of species, phases, and (pure) substances to the conceptual notion of element? The latter finds its empirical base in the periodic system and the existence of (simple) substances that cannot be separated into other substances, except under the most extreme conditions. There seems to be consensus concerning Paneth's (1931) proposal to distinguish basic and simple substances.[84] The *Grundstoff* or basic substance (or element) is "*the indestructible stuff present in compounds and simple substances*"; the *einfacher Stoff* or simple substance is "*that form of occurrence in which an isolated basic substance uncombined with any other appears to our senses*" (p. 129-30, emphasis original).[85] The latter is a chemical substance like others, except that it cannot be decomposed (further) by chemical means. The former provides the basis for the systematic ordering of the elements in the periodic system.[86] Basic substances are the (unobservable) ultimate constituents of matter, whereas "the concept of basic substance as such does not in itself contain any idea of atomism", as Lavoisier acknowledged (Paneth 1931, p. 133). A similar distinction can be made for pure substances (a conceptual notion) and their approximate preparations in the laboratory or the chemical industry. However, it is less clear how this distinction would work for other materials, such as non-stoichiometric substances (unless the latter are categorically stipulated to be substances 'with defects'). Paneth, following Kant (Ruthenberg 2010), speaks of the basic substance being transcendental.

Ruthenberg (2009, p. 89) rephrases this as: "Basic substances are non-observables and rather concepts than concrete objects. They are not bearers of properties." Hendry (2012a), Scerri (2009), and others will say that the atomic number (read: charge of nucleus) is a 'real property' of basic substances.[87]

According to Paneth, a simple substance may occur in different forms (isotopes, allotropes).[88] To some this is counterintuitive. If we use the phase diagram as criterion (classical phase transitions, critical point) than isotopes are different substances. Properties of hydrogen and deuterium, such as triple point, are not the same.[89] The situation for allotropes (as distinct from isotopes) is less clear. Allotropes are different forms of the same basic or simple substance. Today there is a zoo of different kinds of allotropes for elements such as carbon and sulphur. Usually allotropes are different phases, but different allotropes may be different species in the same phase (for example S_2 and S_3 in the gas phase). Sulphur also has many named forms that are mixtures of 'pure' allotropes.[90]

The appearance of carbon has different complexities. There are numerous fullerenes.[91] Although fullerenes are considered allotropes of carbon, diagrams for 'traditional' carbon and fullerene phase diagrams are studied in unrelated ways. Both contain allotropes connected by first order phase transitions at high pressures. Each fullerene behaves differently in column chromatography. The method of preparing 'pure' C_{60} is not fundamentally different from preparing ordinary 'pure' substances. The conversion of C_2 into C_{60} and back looks more like a chemical transformation (changing chemical bonds) than a phase transition.[92] On the other hand, fullerenes have been converted to diamond by applying solely high pressures.

The different forms of sulphur and carbon may be classified in terms of species and phases, but considering them as allotropes is problematic. There is also such a thing as 'chemically induced phase transition'. Such cases undermine a strict distinction between chemical transformations and physico-chemical phase transitions.

Ozone is considered an allotrope of the chemical element O. However, the transformation of oxygen into ozone and vice versa is considered a 'chemical equilibrium', not a phase transition. Oxygen and ozone each have their own allotropes and molecular species.[93] Each survives its 'own' phase transitions while preserving its individuality.

Again we see that the variety of substances is enormous. The notion of 'simple substance' seems simple, but the variety of isotopes, allotropes, and other forms of simple substances leads to many unsatisfactory conventional definitions, as the above examples of S, C, and O show. There are many different ways of 'elements/atoms' binding with itself (*e.g.* O_3, S_3, C_{60},) and the elements themselves turn out to be mixtures of various isotopes (*e.g.* D and

H). And there is more: ions, (free) radicals,[94] and more esoteric phases and species. We have to accept that the variety of chemical substances cannot be fit into a streamlined classification system, whereas the variety is only increasing as the world is extended to more esoteric boundary conditions (extreme pressures and temperatures).

6. Making new things

In modern Chinese the word for chemistry is *huaxue* 化学, literal translation: 'science of material change'.[95] This fits chemistry in the broad sense very well. The most unique kind of transformation, sometimes considered the defining characteristic of chemistry, is synthesis. Synthesis is central to organic, polymer, inorganic, organometallic, and solid state chemistry and is usually associated with chemical reactions taking place. However, preparing heavy water (D_2O), or Helium-4 and Helium-3 isotopes, is also the result of transformation of substances, although no chemical reactions occur.[96] Synthesis is typically followed by purification or concentration (van Brakel 2012c), which also requires further transformations, not involving chemical reactions.

Synthetic chemistry is a unique science in that it produces the objects it investigates.[97] Unlike other branches of science, the scientific products of synthetic chemistry are not merely ideas, but substances that change the material world, for the benefit or harm of living beings. "Rather than depicting the world as it is, chemistry develops an understanding of the world by changing the world" (Schummer 2010, p. 177). Chemistry, apart from being descriptive like other sciences, is also productive, but not in the same way as most of technology (as I already argued in Section 3). But it has also been suggested that new chemical substances or species are *theoretical* entities, because they are postulated by a theory (of molecular structure).

The discourse of chemical synthesis is primarily one of chemical species. However, most of the time the result of species transformation is of little use if the new products cannot be isolated and concentrated as pure substances by separation methods (as in pharmaceutical technology).[98]

Because the changes are radical in that they create *new* stuff, synthesis increases the complexity of the world. Because further synthesis has no limits, chemical knowledge is fundamentally incomplete or "unfathomable" in a way not true of other sciences. The synthesis of new substances increases the scope of possible knowledge (the number of undetermined properties) much faster than the scope of actual knowledge (the number of known properties).[99]

Traditional philosophers usually claim priority for entities, things, or substances and consider changes secondary attributes. In chemistry change is essential rather than secondary.[100] It is essential, because through chemical reactions all substance properties change. Multiple processes are taking place on different time scales. In the natural world there are no fixed and isolated chemical substances, but only permanent chemical change of matter. Chemical species are undergoing continuous (reversible or irreversible) transformations. Interatomic distances and angles are dynamic entities. This suggests that process philosophy might be more suitable for the philosophy of chemistry (Stein 2004, Earley 2013).[101] Process philosophy considers entities only as temporary states. Process philosophies focus on continuing, ever-present change. Process philosophy also fits a stuff perspective better.[102]

The phrase 'chemical space' has not been clearly defined, but its intended meaning is straightforward. It is used in contrast to space-time and 'contains' substances/species and their relations (*i.e.* all possible chemical changes). Seen as a (nonlinear) network, chemical space in the narrow sense consists primarily of 'classical' pure stoichiometric substances at the nodes; the relationships between the nodes are chemical reactions correlated to experimental practice (including reactions with as yet non-existing substances).[103]

Thus (pure) substance identity is dependent on its relations to other substances (Bernal & Daza 2010). Phases, species, and substances can be correlated to one another in some places in chemical/material space. Species and substance interaction is the most noteworthy feature of the relational structure of chemical space, but material space should also include the relational structure of (pure) phases and their transitions. Synthesis and phase theory can provide data for the construction of material space, which ideally should include:

(1) pure (simple and compound) substances and corresponding phase diagrams, allotropes and polymorphs, as well as the many corresponding species (many of which are not known);

(2) non-stoichiometric compounds and solutions of pure substances, as well as the corresponding phase diagrams and species not included above;

(3) species not contained in the above, which may only exist in solution with extremely low concentration and/or having a brief lifetime;

(4) any remaining phases;

(5) all transformational relations between substances/species/phases mentioned above.

Material space is restricted to homogeneous materials. Inhomogeneous materials can be characterized in terms of their constituting phases. Because there are three basic categories (phases, substances, species), there will be many fuzzy boundaries and pragmatic choices in the construction of material space.

For example, each of the following has to be fitted into the space of pure substances,[104] species, and phase diagrams: polymorphs, allotropes, polymers, isotopes, enantiomers, racemates, tautomers, inclusion complexes, addition compounds, and more.[105] Much work needs to be done to provide a more precise and detailed account of the structure of material space.

Chemical or material space requires sophisticated semiotics to name its contents.[106] The semiotics of classification is not unique to chemistry. However, given the huge size of chemical space, one may argue that here we have a case of 'transformation of quantity into quality'. Chemistry can certainly claim the importance of classificatory concepts as a respectable notion in the philosophy of science. It may be noted that the 'rational' classification of the millions of organic substances is impressive, but there are many other classificatory issues in chemistry. In inorganic chemistry and materials science, there are many irresolvable vague boundaries.[107] The impossibility of devising a strictly 'rational' ordering is already illustrated by the unending list of proposals for alternative representations of the Periodic System.[108]

Criteria to identify and divide natural kinds include similarities variously defined (such as similar appearance, projectable predicates, microstructurally defined 'essences') and also origin (causal-historical criteria), but it is not obvious that such criteria will distinguish natural from other kinds (van Brakel 1992a). What is certain about (pure) chemical substances is that they are *not* natural. Simple substances and compounds fail any natural kinds test (isotopes, allotropes, polymorphs, *etc.*).[109] Chemistry does not support essentialist realism as already noted in Section 3. Whether we focus on macro- or micro-description, the alleged essences vary with circumstances (van Brakel 1986).

The fact that chemistry is in the business of making new stuff requires a major change or elimination of philosophical theories of natural kinds. With respect to chemical substances there is no principled difference between natural and artificial kinds (Bhushan 2006). There is no scientific way to distinguish between natural and artificial substances, in contrast to artifacts in technologies.[110] In chemical technology it makes no difference whether the incoming substances are natural or artificial.[111] All stuff originates in the natural world. There is no creation *ex nihilo*. But in principle every (stable or metastable) phase, substance, and species can occur in nature as well as being made by chemists.[112] Somebody might say that chemistry loses the status of science if it has no natural kinds. But a better view is that the notion of natural kind is outdated (also with respect to other sciences).

7. Interdiscourse relations chemistry – physics

By now there is a wide range of studies concerning the various difficulties of relating molecular structure to quantum mechanics. Different authors present their views differently, but almost all agree that 'chemistry' cannot be 'reduced' to quantum mechanics. Here is a selection of remarks, often repeated by many authors.[113] Many chemical concepts, in the first place chemical bond and congeners, are not amenable to quantum mechanical treatment. Covalent and ionic bonds cannot be separated in exclusive concepts. Hybrid orbital representation does not fit into quantum mechanics. Quantum chemistry is incapable of dealing with a *range* of molecules in terms of *one* theory. Selection of trial wave functions is a critical hurdle for quantum treatments of molecules (Woody 2012, p. 431). The existence of isomers and in particular chirality is not to be found in quantum mechanics (Bishop 2005, 2010). According to quantum mechanics molecules do not have a shape (Ramsey 2000). Exact Coulombic Schrödinger equations should be spherically symmetrical, but polyatomic molecules cannot be spherically symmetrical (Hendry 2010a). Electronic configurations for atoms and molecules, the aufbau, Hund, and Pauli principles have not been deduced from quantum mechanics (Scerri 2007b, p. 74). The length of periods in the Periodic Table cannot be derived from quantum mechanics.[114]

Quantum chemistry "cannot even compete with chemical structure theory" (Schummer 2010, p. 171).[115] Molecular structure is imposed rather than explained. The widely used Born-Oppenheimer approximation presupposes a rigid nuclear structure for molecules; the molecular back-bone central to classical chemical structure theory is put in by hand. And perhaps more fundamentally: The notion of molecular *structure* conflicts with Heisenberg's uncertainty relation. Electrons are assumed to move quantum-mechanically, but not the nuclei. Indistinguishability of identical nuclei do not provide a basis for a quantum theory of chemistry (Sutcliffe & Woolley 2012b, p. 422). The whole, its parts, and its environment [form] a high-relational network (Llored 2012, p. 271). If two particles are 'entangled', the quantum state of each particle cannot be described independently.

Bogaard (1978) already made most of these observations in a paper presented at the 1978 meeting of the American *Philosophy of Science Association*. The most detailed philosophical defense of a form of reduction of chemistry to physics by a philosopher, based on Nagel's views, is Hettema (2012a),[116] but he also says:

> The original aim of deriving chemistry from physics without any auxiliary or ad hoc assumptions has not been fulfilled. [Hettema 2013, p. 338]
>
> The transition state as a unique sort of molecule, explicitly adds insights from the reduced theory to the reducing theory. [Hettema 2012b, p. 25]

> The system is assumed to be isolated from its environment in the sense that the environment can be treated classically. [Hettema 2009, p. 151]

> The explanation of chemistry by physical theory has many complications, and the physical foundations of chemistry are found in a multitude of physical theories, patched together with assumptions, approximations and special applications. [Hettema 2012a, p. 2]

Nagel's 'heterogeneous reduction' is not much different from non-reductive stances.[117]

Of course, one cannot *prove* that reduction is impossible, but I do not know of any proposals to derive molecular structure (and explanations based on it) from quantum mechanics *without* making fundamental presuppositions and/or approximations that are external to the discourse of quantum mechanics. For example, the well-known work of Bader, placing chemistry squarely in the realm of physics, is based on the presupposition of a "return to Dalton's notion of an atom as a bounded space-filling object", which postulate is not part of quantum mechanics (Bader & Matta 2013, p. 256; original in italics).[118]

Historically, chemistry and physics kept their disciplinary focus, notwithstanding many interdisciplinary exchanges. The importance of quantum mechanics for chemistry is not disputed. An increasing number of facts can be explained and/or predicted by applying quantum mechanics to a *given* molecular structure. It is not denied that methodological reductionism is a fruitful research program in the natural sciences and perhaps elsewhere.[119] However, typically the reduction of chemistry to physics is presupposed and on this basis the notion of reduction is adapted and made flexible so as to comply with the postulate. Writers in the philosophy of science often take for granted that there *must* be reduction. Confronted with the complexity of the relation of physics and chemistry in quantum chemistry, they modify the definition of reduction (Lombardi 2013).

Surely, physical laws posit restrictions on what can happen in the world, including the chemical world, but leave open many possibilities.[120] Chemical behavior cannot violate the boundaries set by the fundamental laws of quantum mechanics (and relativity theory); the latter provide an *a priori* space of possibilities for chemistry. But which possibilities are actual cannot be derived from quantum mechanics (if only because of the contributions of boundary conditions to actualities).

Unfortunately, there is quite some repetition in the 'anti-reductionist' literature in the philosophy of chemistry and not all writers understand everything they borrow from earlier sources. Woolley (1978) has been cited over and over again, although sometimes his view is not well understood and some authors do not seem to know of more recent publications of the same author (and Sutcliffe). It may be useful to cite Sutcliffe and Woolley at some length to bring out their nuanced view.[121]

> [The] *qualitative* modification of the internal Hamiltonian, the extra choice of fixed nuclear positions in the 'electronic' Hamiltonian, is *ad hoc* [...]. An essential feature of the answer is put in by hand. [Sutcliffe & Woolley 2013, p. 33]
>
> In our view it is not at all evident that the Coulombic Hamiltonian *on its own* will give rise to the chemically interesting features. [...] In other words one should not expect useful contact between the quantum theory of an *isolated* molecule (which is what the eigenstates of the Coulombic Hamiltonian refer to) and a quantum account of *individual* molecules, as met in ordinary chemical situations. [Sutcliffe & Woolley 2012a]
>
> That said, the conventional account, treating formally identical nuclei as identifiable particles when it seems chemically prudent to do so, has enabled a coherent and progressive account of much chemical experience to be provided. But it is not derived by continuous approximations from the eigensolutions of the Schrödinger equation for the molecular Coulomb Hamiltonian, requiring as it does an essential empirical input. [Sutcliffe & Woolley 2012a]
>
> We have never claimed that molecular structure cannot be reconciled with or reduced to quantum mechanics, or that there is something 'alien' about it; our claim is much more modest. We do not know how to make the connection; our hunch is that no-one else does either. [Sutcliffe & Woolley 2011]

They conclude that it is "plainly ludicrous" (Sutcliffe & Woolley 2012b, p. 422) to claim either that quantum mechanics or the idea of molecular structure is wrong. Instead "some new idea is required" (*ibid.*, p. 423). Of course they are thinking of a new idea in chemical physics, but new ideas are equally needed on the philosophical side.

Note that Sutcliffe and Woolley leave open the possibility that some day molecular structure might be derived from pure quantum mechanics. Already, 'Beyond the Born-Oppenheimer Approximation' methods have been proposed, for example by Tapia (2006), who points out that the conclusions of Sutcliffe and Woolley are based on the Coulomb Hamiltonian and claims that in his approach the problems Woolley and Sutcliffe raise do not arise. Whether approaches not taking the Coulombic Hamiltonian as its starting point can avoid adding *ad hoc* assumptions, remains to be seen.[122]

In passing it may be noted that already in physics there is emergence and context-generated ontology all over the place. Physics cannot be reduced to physics (the 'zeroth step'):

- failure of strict reduction in particle physics;[123]
- reduction of classical physics to quantum physics is problematic;[124]
- thermodynamics cannot be reduced to statistical mechanics.[125]

When mentioning extra assumptions required to make quantum mechanics applicable to chemical systems, it is important to distinguish assumptions that find their home in classical physics (*e.g.* collision theory) or classical chemistry (*e.g.* molecular structure). Although it seems certain that quantum chemistry cannot be reduced to quantum physics as it exists today, this is less obvious if classical physics is added to quantum mechanics (Bishop 2010, p. 171). Classical physics provides notions of space, shape, mechanics, and thermodynamic parameters. Also Hettema (2009, 2012a) suggests that chemistry can be reduced to quantum *cum* classical physics.

Most discussions on interdiscourse relations (such as reduction, supervenience, emergence) situate themselves in the philosophy of mind (focusing on the relation between mental and physical or neurophysiological predicates), followed by the philosophy of biology (genotype and phenotype, distant and proximate causes) and philosophy of social science (individuals and the regularities in economics and social science).[126] Philosophy of chemistry cannot merely contribute interesting case studies, but the relation of chemistry with physics (and on the other hand biology) is unique in the sense that if reduction of chemistry to physics fails (or reduction of biology to chemistry), this undermines all reductive forms of physicalism or naturalism in whatever domain in one fell swoop.[127] The relation between chemistry and physics is *the* crucial step for claiming a hierarchy of sciences or any other general type of interscience relation.[128] In addition, the relations between chemistry and physics provide the most detailed and concrete case studies that would have to fit any proposed form of reductive or non-reductive relations between sciences.[129]

Of course, to speak of 'the relation between chemistry and physics' is nonsense (van Brakel 2003, table 1): a whole variety of possible intertheoretical relations have to be addressed.[130] There is no *a priori* reason why the nature of the interdiscourse relation (covariance, dependency, accommodation, reduction, emergence, supervenience, mereological relationships, theoretical identities, intertheoretic approximation, explanatory unification, what have you) is the same for:

- the relations between molecular structure and quantum-mechanical systems of charged particles;
- the relations between macroscopic substances and their constituent microspecies;[131]
- the relations between vernacular and scientific use of substance names;[132]
- the relations between (chemical) thermodynamics, irreversible thermodynamics, statistical mechanics, and quantum mechanics.[133]

The more specific relations in each of these groups may display different interdiscourse relations as well.

As an alternative to a hierarchy of levels connected by reduction or emergence (or supervenience) relations, I propose a form of event monism, which allows a greater variety of interdiscourse relations (including blending or amalgamation – see below). Different disciplines and theories at different levels in these disciplines can be thought of as describing events (including situations, states, processes). Events are pre-theoretic manifest taken for granted entities.[134] Objects are theoretical notions. Different disciplines/theories may claim to describe what, colloquially speaking, is the same event;[135] for example the event of boiling water or an event involving particular chiral molecules. Because identification conditions of events are discourse-dependent, different discourses are strictly speaking not describing the same events, in particular if these discourses focus on different 'levels' (*cf.* Ramsey 1997, p. 237). This kind of incommensurability need not bother us. There is no need for the assumption that the chemical world coincides in an ontologically strict sense with the physical world. A chemical electron may be different from a physical electron. The manifest 'this, here' (including sophisticated instrumentation) connects the different discourses, confirmed by the predictive success of the joint effort of discourses and whatever interdiscourse relations prevail. The latter provide the heterogeneous basis for the unification of science.[136]

In the philosophy of mind and elsewhere, when multiple realization causes trouble for hoped for reductive relationships, one most often resorts to one of the many *asymmetrical* supervenience definitions. But this approach does not work in the philosophy of chemistry. If a sample is a species of water, it must be a cluster of H_2O species, and if it is a cluster of H_2O species it must be a species of water (where the cluster and species are specified as far as current knowledge allows). This would be a *symmetrical* supervenience (or covariance) relation. On the other hand, the relation between molecular structure and charged particles described quantum mechanically, is multirealizable in the wrong direction.[137] As it happens, philosophers of chemistry discussing supervenience always give examples of the relation between macroscopic features such as 'being water' or 'smell' and molecular structure.[138] Supervenience is rarely mentioned as applicable to chemistry and quantum mechanics (but emergence and downward causation is).[139]

Philosophy of chemistry can highlight the need for investigating symmetrical interdiscourse relations and reverse multiple realization. Woody (2012) made the important suggestion that quantum chemistry amalgamates concepts from quantum mechanics and molecular structure theory (and other physical and chemical concepts).[140] Woody writes (2012, p. 459):

> Underneath the diagrammatic and graphical representations themselves rest amalgamated theoretical concepts developed through a complicated grafting of

> quantum theory, classical structure theory in chemistry, and particular mathematical approximation techniques.

A major example of an amalgamated concept is an orbital diagram, a genuinely hybrid representation, neither straightforwardly qualitative nor quantitative, but vital for chemical reasoning. The notion of an orbital derives from quantum mechanics, but in its sophisticated diagrammatic forms has absorbed much of classical chemistry.

The intuition that we should not always think of reductive or emergence relations between two discourses, but of 'fusing' or 'blending' of different discourses is apparent from a range of terminology used by different authors. Harré (2006, p. 509) speaks of *complementary* descriptions; as did Primas before him: A full account requires the simultaneous articulation of complementary modes of description, interconnected by dialectical thinking (Primas 1983, pp. 355, 326). Others speak of the *combination* of classical molecular structure with the quantum properties of the electron.[141] Hettema refers to quantum chemistry as "in between" physics and chemistry, involving "a lot of theoretical and ontological 'borrowing'" (2002a, pp. xvii-xviii).

The amalgamation of concepts is not unique to chemistry. It is widespread in the sciences and its importance is underestimated by purely philosophical discussions of a few interdiscourse relations.[142] Also here philosophy of chemistry could play a central role because of the abundant detail available.

Perhaps the amalgamation model should be applied to the relation of the macroscopic and the microstructural as well. In practice these discourses are intimately mixed.[143] For example, the polywater episode shows how descriptions at different levels are all assumed to describe the same pre-theoretical events and between them resolve the paradoxical observations and speculations (van Brakel 1993). This may well apply to all cases of interdiscourse relations broadly conceived.

The physical and chemical world, themselves patchworks of the many worlds scientists are making,[144] are connected by a range of interdiscourse relations, not necessarily all of the same type.[145] Symmetrical interdiscourse relations, reverse multiple realization, and amalgamation of concepts are central issues for how everything fits together and requires a form of event monism, to which philosophy of chemistry can make important contributions.

Finally, in connection with quantum mechanics it should be noted that there is only (approximate) global supervenience of the special sciences on the physical (and of parts of physics on other parts of physics). A consistent description of any phenomenon in quantum terms must strictly speaking include the entire universe. This might offer support for global supervenience, but it leaves no room for local (or 'weak') supervenience.[146] Quine (1978) writes:

> Nothing happens in the world, not the flutter of an eyelid, not the flicker of a thought, without some redistribution of microphysical states. It is usually hopeless and pointless to determine just what ones supervened in the event, but some reshuffling at that level there had to be; physics can settle for no less.

This is correct, but characterizes global supervenience, not supervenience as usually discussed.

8. Conclusion

Philosophy of chemistry should annex (large parts of) physical chemistry, chemical physics, materials science, geology, and molecular biology.

As elaborated in Section 2, the era of the neglect of chemistry in the philosophy of science is not yet over. It will take some time before substantial articles in philosophy of chemistry will be routinely included in overviews of general philosophy of science. The publication of articles in the journal *Philosophy of Science* and other mainstream journals in analytic philosophy, as well as Elsevier's Handbook *Philosophy of Chemistry*, is a good step forward, and philosophy of chemistry can take advantage of the current concern to include several/many sciences in overviews.

It has been suggested in several places that the philosophy of chemistry has reached its mature stage. There is little doubt that philosophy of chemistry as an autonomous discipline with two international journals is there to stay, but it has not yet reached what one might call a 'critical mass'. A critical mass is reached when there are a few chairs/institutes 'institutionally' dedicated to philosophy of chemistry.[147] Only then will there be sufficient space for Ph.D.'s in philosophy of chemistry to continue their research career in philosophy of chemistry. The existence of philosophy of chemistry still depends very much on contingent factors such as the interests and academic career of particular individuals.

Many subjects in the philosophy of chemistry require a revision of the dominant views on major themes in the philosophy of science and support what are presently marginal positions in the philosophy of science, for example van Fraassen's proposal for a pragmatic notion of explanation, or Cartwright's dappled world and *ceteris paribus* laws. The latter examples suggest empiricism. At the same time, the constructive side of chemistry (making new stuff) provides strong pragmatic support for a realist position. Hence one might speak of a form of constructive realism (which is not much different from van Fraassen's constructive empiricism) being supported by philosophy of chemistry.

If chemistry were the ‘first science’ in philosophy of science, this would involve the following major changes in the philosophy of science (and spin-off in analytic metaphysics, including the philosophy of mind).

(1) Focus on explaining the great variety of materials and their relations, instead of focus on reduction of everything to the one underlying matter of atoms or fundamental particles.
(2) Focus on change (synthesis, transformations, transitions) instead of description of the world ‘as it is’.
(3) Focus on the details of the relations between chemistry and physics may teach us more about the ‘unity of science’ then imposing a hierarchical reductive structure.
(4) Philosophy of chemistry may provide important contributions to the question, ‘How does everything fit together in the world(s)?’ For example, by developing a form of event monism and investigating symmetrical supervenience relations, reverse multiple realization, and the ‘emergence’ of amalgamated concepts.
(5) A completely new theory of kinds is required, dropping the alleged distinction between natural and artificial kinds.

Notes

[1] Categories are not (natural) kinds; they come before any classification. According to Bachelard the notion of (chemical) substance “operates effectively as a *category*” (1940, p. 44). Categories provide a meta-conceptual scheme providing the basic structure of the world (as in Aristotle’s and Kant’s categories). It is not easy to envisage discussing alternative categorical schemes (Derrida 1982).

[2] In contrast chemical physics is usually considered part of physics.

[3] Production of materials that do not involve chemical transformations or physico-chemical phase transitions are not included, for example metamaterials. Metamaterials are artificial materials engineered to have properties that may not be found in nature.

[4] I am indebted to the many publications of Joachim Schummer. These publications present the first and most comprehensive philosophical analysis today of the nature of chemistry. See, in particular, Schummer 1995, 1996, 1997a, 1997b, 1998a, 1998b, 2001, 2003a, 2003b, 2006a, 2006b, 2008, 2010.

[5] A substantial part of this Section is taken from van Brakel 2012a, pp. 39-42.

[6] Immanuel Kant went so far as to suggest that chemistry can serve as an analogy, metaphor, or paradigm for the method of critical philosophy. Cf. Lequan 2000, pp. 5, 105-7 and citations from Kant in note 33 of van Brakel 2006, p. 84.

[7] See for references van Brakel 2000, p. 138. These proceedings may be considered an inventory of issues in philosophy of chemistry already dormant among chemists and philosophers before the 1990s.

[8] The more recent *Philosophies of the Sciences* (Alhoff 2010) contains Schummer 2010.

[9] Although the chemical revolution (from phlogiston to oxygen) has been heralded as Kuhn's primary motivation for his views on the structure of scientific revolutions, in the past decade critical voices have suggested that Kuhn's general theory of scientific revolutions does not fit the particular case of the chemical revolution very well (Blumenthal 2013).

[10] Cf. Klein (2012), who argues that modern chemists' interest in pure chemical substances does not presuppose a concept of pure science.

[11] Important concepts that warrant analysis include: chemical bonding, orbital, hybridization, functional group, electronegativity, substituent effect, configuration, resonance, aromaticity, chirality, acidity, transition state, phase transition point, phase (rule), to name but a few.

[12] Not surprisingly the mostly discussed concept is chemical bonding, but, as yet, there is little synergy. See, recently, Hendry 2008a, 2012b, Needham 2014, Vemulapalli 2006, Weisberg 2008, Woody 2000, 2012. The assumption of a bond between only two atoms is obviously wrong, but rarely addressed (I owe this observation to the late Krishna Vemulapalli).

[13] Mulder (2010) has argued that orbitals are states, not entities.

[14] Adjectives used to modify scientific realism in the philosophy of chemistry include: structural, strategical, operational, constructive, pragmatic. Bensaude-Vincent (2008) has shown that the realism/positivism dichotomy in the philosophy of science overlooks the making stuff feature of chemistry.

[15] Kripke also claimed there to be the existence of contingent and *a priori* statements, for example the definition of the 'standard metre in Paris'. For discussion and critique see van Brakel 1990.

[16] These later publications include: Needham 2000, 2002, 2008ab, 2011, 2014, Ruthenberg 2012, van Brakel 1997, 2005, VandeWall 2007, Weisberg 2006. Perhaps the message still needs repeating in order to educate philosophers.

[17] The problem of bridging connections between systems across widely separated scales is well-known from the philosophy of physics. Modeling shape does not only play a role in the 'reduction' of molecular structure, but also in modeling geometrical boundary conditions in chemical engineering (van Brakel 2012c, pp. 541-2).

[18] For example, according to Bensaude-Vincent *et al.* (2011, p. 375), the periodic system is "the inscription of the basic building blocks that are used by nature and simultaneously the revelation of a unique and general law governing the irreducible diversity of chemical phenomena".

[19] A characteristic of chemistry is the use of non-numerical and discrete mathematics. See Balaban 2005 and the special issues of *Hyle* on 'Chemistry and Mathematic' (2012, no. 1; 2013, no. 1).

[20] Christie & Christie 2000, van Brakel 2000, ch. 6; cf. Vihalemm 2005, Harré 2012.

[21] One might suggest that chemists use "the detour of the laboratory to access nature" (Bensaude-Vincent 2009, p. 168).

[22] Hunger 2006, van Brakel 2000, chs. 6-7; Weisberg 2004, 2012.

[23] See van Brakel 2012c. Vessels, columns, tubes, and other containers have been made to narrow specifications; hence phenomenological equations can be applied

under relatively simple boundary conditions. Although the internal geometry of a unit operation can be highly complex, approximate '*ab initio*' calculation may still be a possibility. However, one cannot avoid multiphase heterogeneous systems in almost any unit operation or sophisticated chemical reactor, and then the geometry of the phase boundaries quickly becomes intractable, in particular if more than two phases are involved. In the chemical industry fitting a model is a matter of mutual attunement of model and 'made reality'.

[24] See Earley 2006, 2008, Harré & Llored 2011, 2013, Llored 2012, Needham 2010a, Sukumar 2013.

[25] Ethyl alcohol (CH_3CH_2OH) has five hydrogen centres. Those hydrogen atoms are not all the same.

[26] Earley (2006) has discussed the features of 'chemical coherences' (dissipative structures, self-organizing collections, open systems) and considers them chemical 'substances', but not 'chemical substances'.

[27] See Goodwin 2009b, 2010, Woody 2004, 2012. The role of diagrammatic representation does not easily fit into standard accounts of the relation between two theories or disciplines and the relation of physics and chemistry in particular (Woody 2000, 2004).

[28] The role of structural formulae supports Goodman's (1978) arguments to consider truth a subsidiary of rightness. Goodman will say that a diagrammatic representation can be right but not true. For Goodman rightness is a matter of fitting and working. See Goodman & Elgin 1988, pp. 155-6.

[29] Including causal explanations based on interventions (Llored 2012, p. 271; Ramsey 2008).

[30] Personally I think that theoretical reasoning can only exist within models or formal languages. If this reasoning is to be connected to events in 'the world' it will always require 'approximate' reasoning.

[31] Much earlier Heidegger had already argued that the essence of even *theoretical* physics is that of the technological attitude of representing and controlling (Ma and van Brakel 2014).

[32] Chamizo (2013, p. 167) introduced the term technochemistry for "the activities derived from the chemical experiment". Klein (2005) has argued that since the seventeenth-century, chemistry has been a technoscience *avant la lettre*. On behalf of Latour-type constructivism Nordmann (2006) has suggested that a substance should be conceived as a "stable assemblage". But this can be proposed with respect to all scientific concepts.

[33] Hoffmann 2003, Laszlo 2003, Schummer 2003b, Weibel & Fruk 2013.

[34] Substantial parts of this Section are drawn from van Brakel 2012b.

[35] The notion of phase should be distinguished from the notion of state of matter (or state of aggregation). Diamond and graphite are the same state of matter (solid) but different phases of carbon. There are an indefinite number of phases and only a few, slowly rising, number of states of matter (solid, liquid, gas, plasma, Bose-Einstein condensate, strange matter, ...). The more exotic states of matter do not occur on earth (not even in laboratories). The distinction between states of matter and phases is fuzzy. For example, mesomorphic phases (liquid crystals) and supercritical fluid phases have also been called different states of matter.

[36] Conglomerates are inhomogeneous mixtures of different phases, for example smoke, concrete, or a mixture of water and ice. Conglomerates are a major focus in geology.

[37] However, at the micro- and nano-scale, phase properties may depend on surface tensions and at an even lower scale, the notion of phase becomes meaningless (like other thermodynamic parameters).

[38] Phase predicates should be distinguished from substance predicates (Needham 2007, 2010a).

[39] Amorphous phases can exist in different modifications (polyamorphism). The transformation of amorphous into crystalline phases and vice versa can be reversible or irreversible.

[40] The region near a phase boundary is, strictly speaking, a separate phase. Mesomorphic phases are anisotropic phases intermediate between solid and liquid; gelatine is a common example. Micelles and other aggregates involving surfactants may also be considered mesomorphic phases. Colloids (sol, gel, emulsion, foam) are sometimes considered homogenous solutions, but more commonly referred to as two phases (a particulate phase dispersed in a fluid phase). To characterize naturally occurring petroleum fluids, eleven distinct phase transitions have been identified. The 'phases' of a block copolymer may display microphase segregation in addition to macrophase separation.

[41] See for the phase rule Needham 2012, pp. 281-5; van Brakel 2012b, pp. 201-5, Vemulapalli 2012, pp. 488-91.

[42] For a critical discussion concerning a possibly third criterion for being a pure substance, entropy of mixing, see Hendry 2010b.

[43] An example is the system BaO-TiO_2. It contains intermediate compounds that exist in their own right (having specific applications). $BaTi_4O_9$ and $Ba_2Ti_9O_{20}$ are useful materials in the context of microwave frequency communication. Other intermediate compounds in this system include: $BaTi_4O_9$, $BaTi_3O_7$, $BaTi_2O_5$, $BaTiO_3$ (two polymorphs), and Ba_2TiO_4.

[44] The label 'compound' is short for compound substance, which can be stoichiometric or non-stoichiometric. See on simple substances end of Section 5.

[45] Because one-phase materials miss the substance characteristic of occurring in more than one phase connected by classical phase transitions.

[46] There are other reversible and irreversible phase transitions. For example, there are magnetic transformations (of, say, α-ferrite to β-ferrite), which do not take place at a definite temperature. But it is disputable whether this should be called a *phase* transition. The crystal structures of α- and β-ferrite are the same and the latter may be considered merely a 'form' of the former.

[47] Sea water is a solution. Air is a solution. A mixed crystal is a (solid) solution.

[48] Separation methods are a neglected core of chemistry. The Dutch word for chemistry is *scheikunde,* literally meaning 'knowledge and art of separation'. It has been argued that this is a method utterly different from other modes of analysis known in the empirical sciences (Klein 2008, p. 38).

[49] Cf. chemical space in Section 6.

[50] Cf. the views of Bachelard and Meyerson (van Brakel 2012a, pp. 31-3). Bachelard argued that true chemical substances are the product of *technique*, not materials

found in reality (1940, p. 45). Meyerson argued that a pure substance is an abstraction created by a theory.

[51] For an early, still relevant discussion of problematic cases see Timmermans 1963 (1928) and further van Brakel 2012b.

[52] Allowing that the contents of the bottle will be stable only in a limited range of pressure and temperature.

[53] Crucially, the calibration of spectroscopic techniques may depend on the preparation of pure substances. Different spectroscopic techniques may suggest different structures of the same substance or species.

[54] For example, argonfluorhydride can be formed in a matrix of solid argon, but not separated from this environment.

[55] Excimers (occurring in lasers or plasmas) are molecules which represent a bound state of their constituents only in the excited state, but not in the electronic ground state; for example, the combination of an inert gas atom (Ar, Xe, Kr) and a halogen atom (F, Cl).

[56] Enantiomers or optical isomers are chiral molecules that are non-superimposable mirror images of each other. Chirality also occurs in inorganic systems, for example $[Co(NH_3)_5Cl]SO_4$ is racemic (*i.e.* having equal amounts of right-handed and left-handed enantiomers of a chiral molecule). All handed objects are chiral, but not all chiral objects are handed. An example of a non-handed chiral molecule is $Pt(NH_3)(NO_2)(NC_5H_5)(Cl)(Br)(I)$, with Pt in the center of an octahedron (King 2003, p. 160).

[57] Slater (2005, pp. 31-41) suggests that each of the following questions may be answered 'yes' or 'no': Do enantiomers differ (1) structurally, (2) dispositionally, (3) in kind? He concludes: "if, as a consequence, essentialism must go by the wayside, then so be it."

[58] There is only an extrinsic difference (Le Poidevin 2000). Chirality of molecules supports realism about space. Enantiomerism requires reference to a global property of space.

[59] The ionic compound $^{40}Ar^{35}Cl^+$ may form at high levels of chloride in the plasma of ICPMS (inductively coupled plasma mass spectrometry), thus interfering with the analysis of arsenic, because $^{40}Ar^{35}Cl^+$ has the same mass as $^{75}As^+$.

[60] Almost always the variety of chemical properties is talked about in terms of electrons and chemical bonding. However, this overlooks the nuclei of atoms, which have a "subtle and largely unknown effect on chemical phenomena" (Pagni 2009).

[61] For a general argument claiming that virtually *all* general concepts are family resemblance concepts, see Ma & van Brakel 2016, ch. 4.

[62] Matter in general and its relation to energy and bonding of fundamental particles is the subject of particle physics.

[63] Bachelard 1940, p. 45. See for a discussion of Bachelard's metachemistry Nordmann 2006.

[64] Cited in van Brakel 2006, p. 74. In passing it may be noted that before 1900, there have been many thoughtful philosophers in the Western tradition who defended a form of anti-atomism, including Aristotle and Kant.

[65] It could be argued that atomism was soon undermined by quantum mechanics. If energy is the fundamental stuff of the world (and matter a derived form), this would also be a world of stuff, not of individuals. However, this has not yet

changed the dominance of what has been called pseudo-scientific metaphysics (Ladyman & Ross 2006, p. 17). One might argue that nanochemistry has moved materials science further into the atomistic paradigm.

[66] I use the word 'stuff' in the sense of the German word 'Stoff', which can be understood as (a mixture of) a mass of solid, liquid, or gaseous material, primarily in its unformed state, and derivatively as the material(s) out of which material objects are constructed (whether by nature, engineers, artists, tailors, *etc*.). The stuff a thing consists of is not the same as its parts; stuff discourse is not about things, but about properties of things. See the work of Hacker and Soentgen reviewed in van Brakel 2012b, § 2. The word *Stoff* is usually translated into English either by substance or by material, depending on context. The word *stuff* may be considered the everyday label for the more scientific notion of material, defined as a quantity of matter.

[67] Note that because of the deep disposition to think and speak in terms of individuals or atoms, ordinary language makes it difficult to formulate the stuff view easily. (Discussions about incommensurability could be applied here. What is the meta-language that opposing participants in the discussion should use when communicating?)

[68] It has been suggested that atoms should be thought of as affordances, not as entities (Harré & Llored 2011, 2013).

[69] Properties at the nanoscale may be a function of particle size. In some cases color may be a function of particle size in the micrometer range.

[70] Chad Hansen is the originator of this so-called 'mass noun hypothesis'; see for a brief discussion and references to the relevant literature Ma and van Brakel (2015, ch. 6). By 'ancient China', I refer to the time of Confucius, Laozi, Mozi, Zhuangzi, and Mencius, the 'Spring and Autumn' period and the 'Warring States' period (722-221 BCE). In modern scientific terminology one could contrast starting with the big bang and 'dividing down' or starting with fundamental particles and 'adding up'.

[71] What is said about non-stoichiometric materials in this Section is taken from van Brakel 2012b, §§3, 12.

[72] These compositional formulas are not universally accepted.

[73] However, also in this case it is possible to argue that $Fe^{2+}O^{2-}$ is doped with the impurity Fe^{3+}; three Fe^{2+} being replaced by two Fe^{3+}.

[74] The most common form of non-stoichiometry involves a solid phase/lattice in which some atoms are missing or found in excess in the solid. If another element replaces the missing atoms, also called impurity materials, one may prefer to consider the non-stoichiometric material as a solid solution, an impure substance.

[75] There is no consensus concerning the thermodynamics of 'perfect crystal lattices'.

[76] Perhaps more commonly referred to as $Ar{\cdot}5.67H_2O$. Also clathrates may be non-stoichiometric, because of unfilled vacancies, apparent from writing, for example: M_xSi_{136} ($M = Na, Cs$ with $0 < x < 24$).

[77] Sometimes berthollides ('pure' non-stoichiometric substances) and substances with variable composition are distinguished.

[78] For references to Wald's many publications see van Brakel 2013.

[79] Wald also argued that the choice of chemical space (cf. next Section), ordered in terms of pure substances or species, is a convention. Other ordering principles are possible (although perhaps less practical).

[80] Composites might be understood in the sense of Aristotle's mixts; see Bensaude-Vincent 1998, 2009, Needham 2009.

[81] Intermetallic compounds (Ni_3Al, TiAl) are to be distinguished from interstitial compounds (Fe_3C, Cr_4C). At first the latter were considered solutions.

[82] Chemistry in the narrow sense focuses on chemical substances and species that obey the laws of definite, multiple, and reciprocal proportions.

[83] A sample is a bit of stuff or material; hence also defined as a quantity of matter.

[84] Paneth's simple substance corresponds to IUPAC's "pure chemical substance composed of atoms with the same number of protons in the atomic nucleus". Basic substance corresponds to IUPAC's 'chemical element'. ("A species of atoms; all atoms with the same number of protons in the atomic nucleus.")

[85] Paneth 1931, cited from the 2002 reprint of the 1962 English translation. At about the same time as Paneth, Meyerson distinguished elements taken in their atomic state and taken in their molecular state, a view somewhat similar to Paneth's distinction between basic substances and simple substances (van Brakel 2012a, p. 32). There is no easy translation of *Grundstoff* and *einfacher Stoff*. Cf. Ruthenberg's (2009) critique of Earley's (2009) terminological proposals.

[86] Scerri (2009) and Wang & Schwarz (2009) have proposed to consider free atoms as a category fundamentally different from the notions of basic and simple substance. The periodic system is based on bound atoms, not on free atoms. A free atom in absolute vacuum may be considered the subject of physics.

[87] Hendry (2006a, 2012a) is right to say that atomic number of an atom or element survives all changes, but it is less clear what else does. Other microstructural properties continually change (cf. Earley 2006).

[88] "One simple substance may occur in different (allotropic) forms" (Paneth 1931, pp. 131, 143).

[89] Hydrogen and deuterium have different phase diagrams and critical points. The triple point of hydrogen is 13.96 K. The triple point of deuterium is 18.73 K, which has been proposed as a reference fixing property for defining a point on the temperature scale.

[90] For example, so called plastic sulphur and its crystallization into amorphous or glassy sulphur concerns a mixture of catena sulphur and cyclo sulphur. Such mixed phases of allotropes may also be referred to as intermediate phases. There are polymeric forms of sulphur and other elements, which are called allotropes, but in polymer chemistry, polymerization is considered a chemical reaction.

[91] C_{24}, C_{28}, C_{30}, C_{32}, C_{44}, C_{50}, C_{60}, C_{70}, C_{72}, C_{76}, C_{84}, C_{240}, C_{320}, C_{540}, and more. A large fullerene may encapsulate a smaller one: $C_{84}@C_{960}$, $C_{240}@C_{540}$.

[92] Allotropic (and polymorphic) conversions can be reversible (classically or not) or are irreversible.

[93] $(O_2)_4$ complexes belong to oxygen. $[O_3{\cdot}O_3]$ complexes belong to ozone. According to IUPAC definitions, ozone and oxygen are different forms of the same simple substance.

[94] Free radicals and ions play important roles in chemical reaction mechanisms.

[95] More precisely, *huaxue* may be translated as (depending on context): science of becoming, influencing, (material) changing into, turning into, transforming, converting, digesting, incinerating, melting, dissolving, thawing.

[96] Below a temperature of 2 K, Helium-4 converts into a superfluid. Helium-3 has a different phase diagram and at least two superfluid phases.

[97] For concrete case studies of synthesis see, for example: Goodwin 2008, 2009a, Hettema 2012b, Rosenfeld & Bhushan 2000. The theoretical entity is the model, which the production of the material substance tries to copy.

[98] Drug design (and perhaps what is called retrosynthetic analysis) might be an example approximating a logic of discovery. For a discussion of retrosynthetic analysis see Goodwin 2008.

[99] This paragraph derives from Schummer 2010, p. 176.

[100] Chemical species are dynamic entities and most chemical substances are not in a state of thermodynamic equilibrium (Brazhkin 2006). However, the factor of time is a relatively neglected feature in the philosophy of chemistry (Weininger 2000, p. 147).

[101] Bachelard already stressed, in connection with chemistry, that becoming defines itself underneath being. When substances are in (catalytic) reaction the meaning of words like ‘presence’ or ‘co-existence’ is not clear anymore (Bachelard 1940, p. 55).

[102] Bhushan has argued that neither substance, nor process is needed as a metaphysical requirement, if we accept the particularism of clusters of contingent properties. “We will need to give up essential properties, contingent properties can give us all the stability we need to account for chemical continuity as well as change” (Bhushan 2007, p. 293).

[103] Schummer 1996, pp. 215-23. Substances and reactivities mutually define each other. Each chemical substance refers to all the others; knowing about a chemical substance includes knowing how it is located among other substances and how it behaves in all chemical reactions in which it can take part. An earlier representative of this view is Bachelard.

[104] The separation of simple and compound substances is not fuzzy.

[105] The distinction between inclusion and addition compounds or complexes may be illustrated with the following example. After decomposition of the binary inclusion complex $[Cu(HCOO)_2(H_2O)_2]\ 2H_2O$, it is followed by decomposition of the addition compound $Cu(HCOO)_2(H_2O)_2$. Coordination compounds are a special case of addition compounds. Molecular addition compounds in alloys and mixed salts may have variable composition. Some addition compounds may exist in metastable equilibrium.

[106] It has been suggested that chemical structure theory is more like a rich sign language than a depiction of individual molecular structures (Schummer 2010, p. 172).

[107] An example of classification problems is the confusing terminology concerning guest-host structures. The addition of huge numbers of novel guest-host structures has added to the terminological confusion. Among others, the following expressions have been used differently by different authors, sometimes speaking of a compound, sometimes of a complex, modified by nouns such as: addition, inclusion, adduct, cage, clathrate, cascade, supermolecule.

[108] See Scerri 2007a, 2009, 2012, Wang & Schwarz 2009, and Leach 2013 and many contributions on this theme in the journal *Foundations of Chemistry*.

[109] The elements of the periodic system, understood as conceptual or theoretical notions, might be considered natural kinds.

[110] Nowadays there is such a thing as the chemical production of biological instruments to produce chemical substances with desired biological properties. The boundary between (some) chemical kinds and (some) biological kinds fades away.

[111] The notion of natural materials can remain in the sense that work in the laboratory is engaged in making and characterizing artifacts in order to provide information on 'natural' materials.

[112] This does not apply to some of the esoteric states of matter elsewhere in the universe.

[113] Many more related remarks have been made; most of them already before 2000; see for an overview van Brakel 2000, ch. 5 and for the most comprehensive survey today Hettema 2012a. Since Bogaard 1978 and Woolley 1978, later authors have not added much, except abundant detail.

[114] For all features of the periodic system causing problems for the reductive program see Scerri 2007a, ch. 9.

[115] Earley (2012) pointed out that molecular structure generally depends on contingent historical circumstances of synthesis and separation.

[116] Hettema (2012a) says quantum chemistry is not reductive in the eliminative sense intended by Kemeny and Oppenheim, but it can be reduced in Nagel's sense. The interpretation of Nagel's view is contested. It could be argued, as Nagel seemed to do himself, that the requirement to add 'suitable supplementary principles' (reduction postulates) meant that one cannot really speak of reduction (van Brakel 2000, pp. 51-6).

[117] See Needham 2010, van Brakel 2000, pp. 51-56; 2004. Hettema (2012a) remarks several times that "to a significant degree" reductive and non-reductive views on the unity of science can be reconciled (pp. 56, 251, 296, 404).

[118] See also van Brakel 1997, pp. 267-8. Adherents of QTAIM (quantum theory of atoms in molecules) will say that this criticism is superficial and irrelevant. For a more detailed philosophical analysis see Hettema (2013, p. 324), who concludes that QTAIM does use a number of additional theorems for its construction.

[119] As to epistemological and ontological/metaphysical reductionism, I happen to believe that this distinction cannot be made so neatly as is generally assumed. Cf. McIntyre 1997.

[120] Cf. Vemulapalli 2012, p. 200. This point was already made by Bogaard (1978, p. 348). Cf. Ladyman and Ross 2007, p. 44.

[121] See also Sutcliffe and Woolley 2014.

[122] Decoherence has been suggested as a way to model the 'creation' of molecular structure by the environment. Sutcliffe & Woolley (2011, p. 94) remark "modern formulations under the chic heading of 'decoherence' [... also] start with some primitive notion of structure built in [...] crucial ideas are put in by hand at the outset."

[123] Assume all matter consists of quarks and leptons, but this is still a long way from atoms. For example, the relation of a proton to its three constituting quarks is far from clear.

[124] Information about the classical world has to be used in 'deriving' classical physics from quantum physics (Bishop 2010). In discussing the relation to quantum mechanics, the latter is taken for granted, although nobody knows what the ontology of quantum mechanics is (Lombardi & Castagnino 2010).

[125] Concerning the alleged reduction of chemical thermodynamics and statistical mechanics see van Brakel 2000, §5.2 and the publications of Primas and Sklar reviewed there.

[126] The general philosophical question is: "How does 'everything' fit together in the world(s)?" For some idea of the great variety of interdiscourse relations and alternative definitions of reduction, supervenience, *etc.* see Hendry 2012c, Hettema 2012a, Needham 2010b, Scerri 2007b, van Brakel 1996, 2003, 2010, Vemulapalli 2003.

[127] Denying reduction to physics does not exclude physics being ubiquitous in the sense that it has *something* to say about events in every specific domain (but not *everything*).

[128] Several authors have pointed out that philosophy of mind can learn from the study of interdiscourse relations in the philosophy of chemistry (e.g. Earley 2008, Newman 2008, p. 52).

[129] In addition, philosophy of chemistry provides ideal test cases to compare what scientists actually do with various philosophical proposals of interdiscourse relations (Llored 2012).

[130] Cf. Hettema 2012a, p. 202: each theory is connected with many others in many different ways.

[131] For the complexities of this relation see van Brakel 1986; 2000, chs. 3-4, Primas 1985, Hettema 2012a. For a sustained defense of the microstructural approach to the reduction of substances to molecular structure see Hendry 2008b. In addition there are "entities that are intermediate between the molecular and the substance" (Weininger 2000, p. 154).

[132] On the relation of vernacular and scientific notions of substance, water, acidity, and other chemical concepts see Chang 2007, 2012, Hendry 2012d, van Brakel 1986, pp. 294-6, 305-6). Chang argues concerning the concept of acidity that "the everyday concept is the unifying force that holds together a plurality of scientific concepts." On the vernacular use of water see Ruthenberg 2012 and other papers in that volume.

[133] For example, one might think that temperature is the average kinetic energy of molecules. This is incorrect. It may be true for ideal gases, but not generally, whereas temperature is involved in both equilibrium and kinetic considerations. See Primas 1985; 1991, pp. 163-4; van Brakel 1986, p. 313; 1997, pp. 267-8; Needham 2010. Can the laws of Fourier and Fick be reduced to the equations of irreversible thermodynamics or to statistical mechanics?

[134] For more detail see van Brakel 1999; 2004, pp. 25-7, 30-4; 2010, pp. 123-4, 130-2.

[135] See on the indeterminacy of event identification van Brakel 2004; 2010, pp. 132-3).

[136] Unification can mean many things (van Brakel 2003, pp. 35-6). Consistency is an important feature of unification, but it may be necessary to allow for paraconsistent logic.

[137] As when it is said that quantum mechanics cannot distinguish between (stereo)isomers. According to Le Poidevin (2005), nothing can differ in terms of atomic valency without also differing in terms of electronic configuration. But as

Scerri (2007c) points out, the sulphur atom can display different valences depending on the compounds to which it belongs though there is only one unique 'underlying' electronic configuration. That is to say, multiple realization of the 'lower' level in the 'higher' level.

[138] Harré (2006) uses chemistry/biology as an example of supervenience. Scerri & McIntyre (1997, pp. 225-6) mention smell as an example and Newman's (2008) prime example is water. When supervenience is mentioned in the context of quantum mechanics, no concrete examples are given; only general comments on the difference of reduction, emergence, and supervenience in relation to physicalism (Bishop 2005, Hendry 2010a).

[139] To combat terminological ambiguity, reduction might be defined as the opposite of emergence (van Brakel 2010, pp. 128-30). See for discussion of downward causation and emergence: Hendry 2006b; 2010a, pp. 187-90; Scerri 2007c, 2012.

[140] Amalgamation in this context is to be understood 'exactly' in analogy with its meaning in chemistry (Woody 2012, p. 459f).

[141] Cf. also Bishop and Atmanspacher 2006, Llored 2012.

[142] Blending of concepts into hybrid concepts has also been suggested as an important feature of translation and interpretation across widely different traditions, for example classical Chinese and European languages and traditions (Richards 1932; Ma & van Brakel 2016, ch. 10).

[143] See Vemulapalli 2008, showing the convoluted relations of micro- and macro-discourses when identifying components, substances, and species, or calculating their properties. An absolute and strict separation between macroscopic and microscopic descriptions is not possible and does not make sense.

[144] As philosophers of an empirical bend are well aware, *the world itself* is a posit, which lacks extension except when a particular intensional context is provided (van Fraassen 2002, p. 24). For the plural 'worlds' see Goodman 1978.

[145] A strict separation between different discourses is not needed (and not possible) and primarily serves as a model imposed on a messy world. We should neither speak of unified nor of disunified science, but of a variegated interconnected patchwork (van Brakel 2010, p. 134). I have also referred to it as a "fluid dimensional patchwork" (2004, p. 34).

[146] S weakly supervenes on B if and only if necessarily any two things that have the same properties in domain B have the same properties in domain S (that is, B-indiscernibility entails S-indiscernibility). S globally supervenes on B if and only if any two worlds that are B-indiscernible are also S-indiscernible. There are many paraphrases of 'S supervenes on B'; for example: B underlies S, B grounds S, *etc.* (van Brakel 1996, pp. 255-9).

[147] Cf. also Glymour's (2004) review of Earley 2003a.

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