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Natural Kinds and *Ceteris Paratis* Generalizations: In Praise of Hunches

W. Christopher Boyd and Richard N. Boyd

Abstract: According to stereotypical logical empiricist conceptions, scientific findings are approximately true (or perhaps true *ceteris paribus*) law-like generalizations used to predict natural phenomena. They are deployed using topic-neutral, generally reliable inferential principles like deductive or statistical inferences. Natural kinds are the kinds in such generalizations. Chemical examples show that such conceptions are seriously incomplete. Some important chemical generalizations are true often enough, even though not usually true, and they are applied using esoteric topic- and discipline-specific inference rules. Their important methodological role is to underwrite often-enough reliable, often socially implemented, scientifically informed guessing about chemical phenomena. Some chemical natural kinds earn their naturalness mainly from participating in such generalizations. These results generalize: many scientific generalizations, inference rules, and natural kinds function to inform guessing, that is, to underwrite the generation of hunches.

Keywords: *Natural kinds, chemical synthesis, nominal essences, real essences, scientific hunches.*

1. Introduction: Issues About Representations and Inferences in Chemistry, and in Science More Generally

The legacy of logical empiricism, and of related approaches to the philosophy of science, includes stereotypical conceptions of scientific findings, concepts, and methods that are widely influential when philosophers and scientists examine philosophical questions about scientific practices. We argue that an examination of actual practices of chemists, especially synthetic chemists, makes it clear that these stereotypical conceptions are very seriously mistaken, and we propose some alternative conceptions.

We begin by following M. Christie (1994) and Christie & Christie (2000, 2003) in holding (*pace* Vihalemm 2003, 2005) that important generalizations in chemistry fail to conform to received empiricist stereotypes of laws in science,

especially those in physics. We follow Bhushan & Rosenfeld (2000), Harré (2005) and Bhushan (2006) in holding (*pace* van Brakel 2000, 2005, 2014) that there are natural kinds in chemistry, and we explore questions about their roles in synthetic chemistry. We describe several different ways in which important chemical generalizations differ from stereotypical ‘laws’, and explore their implications for how we should understand natural kinds. We hope to contribute to the sort of pluralism about scientific knowledge represented by the work of Chang (2012) and Hoffmann (2007).

We focus our criticism on stereotypical approaches on four important issues.

1.1 The nature of important scientific generalizations

According to stereotypical empiricist conceptions, important generalizations, at least in mature physical sciences, are universally true ‘laws of nature’, or laws that are approximately true in some specified domain, or mathematically precise statistical generalizations, or even generalizations true ‘*ceteris paribus*’. The models here are the ‘laws of physics’, as empiricist philosophers understood them. We argue, about several types of important chemical generalizations, that they depart sharply from this conception. In particular, the scope of these *non-stereotypical generalizations* differs sharply from what the empiricist stereotype of laws would suggest.

1.2 Scientific ‘rules of inference’

It is part of the empiricist legacy to think that, when scientists infer conclusions from scientific generalizations, they can be thought of as doing so by something like formal rules of inference: deductive logic, justifiable statistical inferences, or the like. In particular, the fundamental inference rules that underwrite scientific inferential practices are thought to be topic-neutral and, thus, discipline-nonspecific. We argue instead that many reliable inferential practices in chemistry are underwritten by informal topic-and-discipline-specific ‘rules’, many of which are not explicitly formulated (or even explicitly formulable) at the time when they are employed. Instead, they are reflections of what we may call the *inferential architecture* of the discipline of chemistry at the time when they are implemented.

1.3 Natural kinds in chemistry

There are many conceptions of natural kinds, properties, relations, magnitudes, *etc.* (henceforth: natural kinds) and of natural kind terms (for overviews see Beebe and Sabbarton-Leary 2010, Kendig 2016, and Slater 2015), but there is a deeply influential, stereotypical conception that many philoso-

phers characterize as the ‘traditional’ conception of natural kinds and of natural kind terms: natural kinds are mind-independent categories that are defined by something like necessary and sufficient membership conditions and that figure in something like fundamental laws. A natural kind term that is scientifically useful can ordinarily be expected to have a very narrowly determinate reference: to exhibit very little referential ambiguity.

On the stereotypical conception, many of the kinds, properties, relations, and magnitudes that appear in non-stereotypical chemical generalizations will not be candidates for being natural kinds, *etc.* We advance an alternative conception and argue that, whatever the merits of the stereotypical conception, the alternative is required to underwrite a scientific explanation of the achievements of synthetic chemists. According to that alternative conception, many of the chemical kinds that figure in non-stereotypical chemical generalizations earn their status as natural kinds, not so much by participating in laws (in the empiricists’ sense of ‘laws’), by having precise boundaries, or by being mind-independent, but by figuring in those important non-stereotypical and discipline-specific generalizations that are implemented by discipline-specific patterns of inference. Their status as natural kinds is discipline-dependent and thus, in an important sense, mind-dependent.

1.4 ‘Context of invention’: Scientifically informed guessing

An historically important aspect of logical empiricist philosophy of science involved distinguishing between the ‘context of invention’ – the factors that underwrite scientists’ invention of theories or possible synthetic procedures, or hypotheses about reaction mechanisms – and the ‘context of confirmation’ – the methods appropriate for testing ideas generated in the context of invention. Philosophy of science was supposed to study only the latter, leaving the context of invention to psychologists and historians. Scientific methods, logical empiricists maintained, involved no ‘logic of discovery’ or ‘logic of invention’, but only methods for evaluating scientific proposals once they were put forward.

We argue that the generalizations, inferential practices, concepts, and natural kinds that depart from the empiricist conceptions have, as one of their central methodological roles, the underwriting of a ‘logic’ (of a sort) of invention. They underwrite scientifically informed guessing about which theories, synthetic procedures, *etc.* are reasonable to pursue, that is, about which hunches to follow. We emphasize as well that this guessing is not only often underwritten by socially constituted inferential architectures, but that it is also often achieved by socially implemented reasoning – by collaborative judgments about what guesses to pursue.

2. Inferential Architecture and the Scope of Chemical Generalizations

For a variety of important chemical generalizations, their appropriate ranges of application differ sharply from those suggested by empiricist conceptions of laws. Often, the syntactic form of a chemical finding will not be a good indicator of its scope of application. Instead, the appropriate scope of application of such a generalization is often determined, not by abstract, formal, topic-neutral rules, but by quite specific features of chemical practice at the time when the generalization is applied.

Some terminology may help here. Cognitive scientists use the term ‘cognitive architecture’ to describe aspects of the systematic ways in which information is processed in human minds or brains. Similarly, computer scientists use the term ‘computational architecture’ to describe basic features of information processing in computers and implemented programs. By the ‘inferential architecture’ of a discipline at a given time, we mean the inferential practices that are central to the practices of the discipline at that time. These will ordinarily include the inferential practices and norms, like formal rules of inference in deductive logic, Bayesian principles of statistical inferences, *etc.* that are featured in logical empiricist approaches. They will also include discipline-specific inferential practices, rules of thumb, experimental and observational practices, evidential standards, *etc.* Importantly, many of these items will not be explicitly formulated in any discipline at the time in question. They will instead correspond to what Polanyi (1969) called ‘tacit knowledge’ and to the tacit aspects of what Kuhn (1970) called ‘paradigms’. They will correspond to reasoning skills that are taught and refined in actual research groups and shared in disciplinary conferences.

For example, a contemporary biologist studying the behavioral ecology of some family of mammals will have acquired in graduate school and later scientific work all sorts of ideas, concepts, reasoning strategies, experimental skills that are peculiar to behavioral ecology and evolutionary biology and to the study of her particular mammal family. She will deploy evolutionary notions like ‘species’, ‘adaptation’, ‘learning’, ‘fitness’, *etc.* that are not fully explicated in her discipline’s literature (or anywhere else), relying on intuitions, trained judgments, perceptual skills, particularly salient examples from the literature, *etc.* In her experimental designs, she will (of course) rely on the best available published finding about her species and on the best available statistical methods, but she will also rely on the unpublished experiences she and other researchers have had in working with the species in question and with related species. These discipline-specific informal principles, rules of thumb, experimental techniques, and tacit understandings are parts of her discipline’s inferential architecture. They are the sorts of things that she went

to graduate school to acquire, that she reads in the literature and goes to conferences to improve, and that she tries to instill in her students.

2.1 Reports of chemical syntheses: Generalizations true *ceteris paratis*

Many reports of successful syntheses are reported in papers with titles of roughly the form ‘The synthesis of X via Y’, or ‘A method for X-ing’, or ‘The X-ing of Y by Z’. The characteristic published content of such papers is a small number of illustrations of chemical transformations of the type in question: some syntheses of some Xs via some Y-ings, or some X-ings achieved the method in question, or the X-ing of some molecules or ions of type Y, carried out by procedures of type Z. Often, some discussion of possible reaction mechanisms for the relevant transformation is included.

The scope of such papers

Almost never is the intended scope of such a paper limited to the reactions reported therein. Instead, the paper will be understood, by its authors and readers, to have more general implications about how chemists can accomplish multi-step syntheses. Here are some examples of papers with a small number of examples but very wide scope implications *ceteris paratis* (we will explain this term in a moment):

- Suzuki-Miyaura cross-coupling (Miyaura & Suzuki 1979): 14 examples. (Akira Suzuki shared the 2010 Nobel Prize in Chemistry for this work.)
- Sharpless asymmetric epoxidation (Katsuki & Sharpless 1980): 8 examples. (K. Barry Sharpless shared the 2001 Nobel Prize in Chemistry for this and related work).
- Evans aldol reaction (Evans *et al* 1981): 6 examples.

Implications ceteris paratis

Although they provide some few examples, papers like these have much broader *implications* for multistep syntheses. The reader of such a paper is invited to try variations on the reported syntheses in her own work. Consider the reader of a paper with a title like ‘The X-ing of Y by Z’. The reader is invited, supposing that she is trying to carry out a multistep synthesis where at one stage a product would be a Y (or have a Y as part of its structure) and she would like to X that Y, to try to use some variations on the X-ing procedures, Z, reported in the paper.

Which variations? Should we understand these broader implications on the model of the implications of laws as logical empiricists understood laws? Do the authors of such a paper intend, or are they understood to intend, to

say that this will *always* work? Surely not. How about most of the time? Surely this need not always be the case: the mechanisms operating in the published reactions might have depended on properties of the particular Ys in question and of the X-ing processes, Z. They might, for example, have crucially depended on the reactions being carried out in an acidic environment that would destroy the intended product in some analogous synthetic attempts, or they might operate only at temperatures at which other prospective products would be too unstable. The contribution of the paper to synthetic chemistry could be profound if the sort of synthetic procedure it proposed works *often enough* to underwrite important synthetic achievements, even if not under most conditions. The reader of the paper is invited to rely on her own background chemical knowledge (which will often be manifested in other non-stereotypical generalization) to identify variations on the X-ing of Y by Z that are plausible for her own synthetic project.

In general, a synthetic paper will have been a significant contribution to the literature as long as the following is true often enough to be useful, even if not *most* of the time: *by fiddling around in a chemically informed way with the procedures indicated in the paper one can carry out analogous syntheses of other products*. Let us elevate this conception to academic respectability by Latinizing it. Such generalizations are true *ceteris paratis* (with other things prepared, *i.e.*, fiddled). They represent one important case of non-stereotypical generalizations in the sciences. Their role is to help underwrite chemically informed *guessing*.

Non-traditional inferences: The role of local inferential architecture

Chemists rely on *ceteris paratis* generalization to inform their guesses about likely synthetic techniques. Do they derive their guesses by deducing them from the contents of the relevant papers? Or by formal principles of statistical inference, or any other topic-neutral inferential procedures? That the answer is ‘no’ can be seen by considering what a scientifically informed person without expertise in synthetic chemistry (a geologist, say, or a particle physicist, or a philosopher of science) could infer from a paper of the form ‘The X-ing of Y by Z’ sort we are considering. If she had taken some chemistry courses that explored synthetic techniques, she might be able to understand the particular instances of the X-ing of some Ys by Z that the paper presents, and the particular mechanisms for them that the paper proposes.

What she would not be able to do, but what a practicing synthetic chemist could do, is to figure out what recommendations regarding new syntheses – what guesses about how to proceed – are understood by the authors, and by synthetic chemist readers, to be conveyed by such a paper. The application of topic-neutral formal principles of inference would not suffice here; she would need to be relevantly immersed in the inferential architecture of synthetic

chemistry. It turns out, we will argue, that topic-specific inferential practices play an important role in the application of other sorts of non-stereotypical generalizations (and of many stereotypical ones as well).

Making cetera parata: How to fiddle things right

In fiddling to adapt the procedures in a published synthesis to her own multi-step synthesis, a chemist will consider, in the light of her chemical knowledge (more on that later), many issues. Such issues include the choice of solvent, temperatures, and additives; order of steps; which protecting groups to employ; how to avoid or create steric hindrance; how to avoid or create conjugated π -systems that reduce reactivity or induce new reactivity, *etc.* Many chemists and philosophers of chemistry will be familiar with some of these issues. We hope, however to make the considerations we offer here accessible as well to philosophers of science without a sophisticated background in chemistry, so we offer, for those readers, an illustrative example of one dimension of fiddling.

Deploying protecting groups

Protecting groups are chemical groups temporarily added to molecules, in the course of a multistep synthesis, to achieve *regioselectivity* in synthetic reactions, that is, to make sure that steps in the synthesis occur only at desired locations in the relevant molecules. Suppose that, at some step in a synthesis, a chemist would like to effect a change at a particular site (call it the *desired site*) in a target molecule – the addition of some functional group for example – via a reaction with some particular reagent. It sometimes happens that the reagent in question would produce an unwanted change at another *undesired* site in the target molecule.

Often a chemist is able to respond to this sort of situation by deploying a ‘protecting group’ at the undesired site. A temporary change is effected at the undesired site – adding a protecting group – via some reaction that leaves the desired site largely unchanged. Then the desired reaction is carried out at the desired site. Finally, the protecting group is removed, thereby effecting the overall change that the chemist seeks.

A chemist’s decision to employ protecting groups in a complex synthesis will ordinarily lead her to rely on many non-stereotypical chemical generalizations. Suppose, for example, that she relies on a paper about the X-ing of Y by Z to make a chemically informed guess about how to X some Y by Z in a step in a complex synthesis. Of course, she will be relying on the *ceteris paratis* generalization implicated in that paper. It will be likely that she will rely on still further *ceteris paratis* generalizations in deciding how to deploy the relevant protecting groups.

Steric hindrance

Steric hindrance occurs when a reaction between a particular site in a molecule and some other molecule is rendered impossible, or impractically slow, because some bulky substituent on the first molecule blocks the second molecule's access to the site. A chemist carrying out a multi-step synthesis may need to avoid or take advantage of steric hindrance at particular steps in her synthesis. If she needs to take account of steric hindrance, she will likely rely on other sorts of non-stereotypical generalizations. Although quantitative predictions of steric hindrance effects are possible, at various levels of theory, synthetic chemists often rely on their chemical training and intuitions, rules of thumb, and pictorial representations of molecular structures to (qualitatively) gauge the probable steric effects of particular molecular substituents. They thus often rely on non-stereotypical general knowledge in assessing the probable effects of steric hindrance.

2.2 Tendency generalizations

Other non-stereotypical chemical generalizations are important in synthetic chemistry. A wide class of such generalizations consists of generalizations that describe useful *tendencies* in chemical reactivity (Xs tend to Y). Such generalizations often depart from the stereotypical conception of generalizations that are something like laws and involve well defined natural kinds. Consider the following two examples:

- The keto tautomers of ketones and aldehydes tend to be favored over enol forms at equilibrium.
- Transition metal complexes tend to be stable with 18 valence electrons in the metal's coordination sphere.

Each of these generalizations is chemically informative and is widely taught in chemistry courses. The second has a rationale in molecular orbital theory for transition metal complexes with regular octahedral symmetry (point group O_h) and six π -acceptor ligands, but it is assumed to be *often* true for complexes with a variety of symmetries, number of ligands, and types of ligands.

On what does the informativeness of these generalizations depend? Are they always true? No, many counterexamples are known. Are they almost always true, or true in the majority of cases? Perhaps, but their informativeness does not depend on whether or not this is so. What makes these and related generalizations informative is that they are true often enough to be useful in the sorts of cases with which synthetic chemists routinely deal. They are very different from the laws that inform the empiricist stereotype of scientific generalizations.

Another sort of tendency generalization illustrates a related point about the kinds that figure in the thinking of synthetic chemists. Electronegativity is an excellent example of an incredibly important concept in chemistry, but one that nevertheless lacks the sort of precise definition anticipated by stereotypical conceptions. The concept of electronegativity reflects the chemically intuitive notion that some elements are more likely than others to bear a partial negative charge in polar covalent bonds. Covalent bonds between two atoms tend to be stronger (*i.e.* more energy is required to break such bonds) when these atoms are of elements that differ in electronegativity. The concept can be extended to apply to functional groups, as well as to elements, and generalizations involving the electronegativity of functional groups play an important role in the ways synthetic chemists think. For example, electrophilic aromatic substitution reactions proceed more or less quickly if there are electron-donating or electron-withdrawing substituents, respectively, on the aromatic ring undergoing substitution. The group electronegativity concept is also useful to inorganic chemists: one can often adjust the electron density at a transition metal atom or ion by adding electron-donating or electron-withdrawing (*i.e.* less or more group-electronegative) organic substituents to the ligands bound to it.

What is important for our purposes is not whether generalizations involving electronegativity do or do not fit the empiricist stereotype of laws of nature. What is important is that the concept of electronegativity altogether lacks a precise definition of the sort that the stereotypical conception anticipates. A number of definitions have been proposed for the electronegativity of elements (see *e.g.*, Pauling 1932, Mulliken 1934, Allred & Rochow 1958). Pauling's definition is the most frequently employed, but there is no chemical consensus about a precise definition of electronegativity of elements. Although attempts have been made to define 'group electronegativity' values for common clusters of atoms, there is likewise no settled definition for those cases either. Chemists rely on trained judgments and intuitions instead. So, generalizations regarding electronegativity, like *ceteris paratis* generalizations and generalizations true often enough, are important in synthetic chemistry despite departing from the stereotypical conception.

The same is true of the next tendency generalization that we will discuss.

2.3 'Hard' vs. 'soft' acids and bases

Another 'tendency' generalization that is important in synthetic chemistry holds that reactions between hard acids and hard bases, and those between soft acids and soft bases, tend to form adducts more readily than do reactions between hard acids and soft bases or between soft acids and hard bases. Pearson (1963) proposed the hard/soft acid/base (HSAB) theory, according to

which the formation of hard acid/hard base adducts and soft acid/soft base adducts are highly thermodynamically favorable, while the formation of hard acid/soft base and soft acid-hard base adducts are less favorable.

Theoretical explanations for this phenomenon have been proposed. According to the most commonly cited explanation, the important factor is a Lewis acid or base's polarizability, *i.e.* the capacity of the electron 'cloud' of a molecule to become distorted in response to electric fields associated with other molecules. Soft acids and bases tend to be significantly more polarizable than hard ones, and this greater polarizability allows soft acids and bases to distort their electron densities in ways that favor the formation of adducts with strongly covalent bonds.

In the case of interactions between hard acids and hard bases, there is less potential to form mainly covalent bonds, but there is enhanced potential to form adducts where the bonding is less covalent, instead being predominantly due to Coulombic attractions. That is because these less polarizable 'hard' acids and bases have greater charge densities at their positive or negative sites, tending to allow for stronger Coulombic interactions between the positively charged portion of an acid and the negatively charged portion of a base. In cases of strong acid/weak base or weak acid/strong base interactions, neither of these factors is present, so there is a diminished tendency towards adduct formation.

The theoretical principles underlying HSAB theory can be handled quantitatively. Drago and Wayland (1965) proposed a parametric equation relating the enthalpy of Lewis acid-base adduct formation to the abilities of the acid and base to participate in covalent ('soft') bonding and noncovalent, predominantly Coulombic ('hard') bonding, and rationalized the form of their equation based on approximate molecular orbital theory. More recently, Ayers (2007) proposed a firmer mathematical justification for the results of HSAB theory. And, of course, the polarizability of a molecule or ion can be calculated using quantum chemistry techniques. So, perhaps, in principle chemists could apply the HSAB conception by deploying theories that fit the empiricist conception of laws. Does this possibility mean that the HSAB conception lies outside the scope of the anti-empiricist approach offered here?

Two things suggest that it does not. In the first place, chemists very often use HSAB theory *qualitatively*, making educated guesses as to a species' approximate hardness or softness in order to predict whether a reaction will or will not be favorable, without using numerical data or making quantitative predictions. The basic generalization about adduct formation is what we have called a tendency generalization, and chemists' successful applications of it often rely on intuitive or informal estimates of hardness and softness. Their successful applications thus do not depend on the categories in question having precise boundaries or numerical specifications or on the application of

strict laws. HSAB theory is an instance of what we suspect is a widespread phenomenon: insightful chemical generalizations whose contributions in practice (*i.e.*, in the discipline's inferential architecture) proceeds mainly by non-stereotypical inference from non-stereotypical rules of thumb, even when more theoretically sophisticated (and stereotypical) approaches may be possible. In this way, HSAB theory is a fertile source of applications of what we have termed non-stereotypical generalizations framed in terms of non-stereotypical chemical kinds.

What makes this case especially interesting is that recently there have been challenges to the received theoretical underpinnings of the HSAB perspective, and to the extent of its reliability as a guide to reactivity. In particular, Mayr *et al.* (2011) argue that HSAB principles are not a reliable guide to the reactivity of organic electrophiles (*i.e.* electrophiles whose electrophilic site is a carbon atom), though they do not argue for a similar unreliability when HSAB theory is applied to reactions of metal electrophiles. If these challenges are correct (we express no opinion), then the contribution that HSAB rules of thumb do still make to the synthetic chemistry of metal compounds is an instance of a non-stereotypical scientific generalization having narrower applicability than once was thought, but remaining quite useful in a more limited domain.

3. Non-stereotypical Natural Kinds

There is a wonderfully rich literature about the existence and nature of natural kinds in chemistry (in addition to works cited earlier see, *e.g.*, Harré 2005; Hendry 2006, 2010; LaPorte 1996, 1997, 2004; Needham 2000, 2002; Van Brakel 2000; Weisberg 2006). A central issue has been the interesting question of the extent to which chemical kinds like elements and particular chemical species are defined along the lines suggested by Putnam's (1975) claim that water is H_2O : whether, that is, they conform to something like the stereotypical conception of natural kinds.

What we have seen is that, whether or not chemical elements and chemical species like water fit the stereotype of natural kinds, the kinds that figure in non-stereotypical chemical generalizations often do not. We propose that a broader conception of natural kinds and of the terms and concepts referring to them is required.

3.1 A broader conception: Natural kinds as contributors to inductive and explanatory success(es)

A number of authors (see, *e.g.*, Slater 2015, Ereshefsky & Reydon 2015, Griffiths 1999, Kornblith 1993, Magnus 2014, Wilson 1999, Wilson *et al.* 2007, Boyd 2010, and Psillos 1999) have articulated conceptions along these lines. There is no consensus about exactly how to formulate the broader conception of natural kinds, but the basic idea is as follows.

The natural kinds (properties, *etc.*) in a discipline, and the natural kind terms and concepts that refer to them, figure in the causal explanation of the epistemic successes of the practices in the discipline: in the explanation of the (typically approximate) reliability of its inferential architecture *in practice*. The definition of a given natural kind term or concept in a discipline will be a set or family of properties such that (1) *given the inferential architecture of the discipline in practice*, the uses of the term or concept tend to reliably track the presence or absence of those properties and (2) that fact, *together with the rest of the discipline's inferential architecture*, contributes to explaining the epistemic successes of practices in the discipline. Any particular version of this basic conception will, of course, fill in more details and will deploy resources for dealing with, *e.g.*, ambiguous or non-referring terms. Four things follow from any version of the broader conception.

First, natural kinds need not figure in laws: their uses can contribute to the reliability of practices when they figure in, for example, generalization true *ceteris paratis* or in generalizations that are approximately true often enough.

Second, their definitions need not establish precise boundaries for the kinds in question. Many versions of this broader conception were designed especially to handle cases of kinds in biology where precise boundaries are not to be expected.

Third, the definitions of a natural kind (property, *etc.*) and its status as a natural kind are relative to the overall inferential architecture of the relevant discipline, including the inferential roles of other terms and concepts in the discipline.

Finally, for just that reason, we should not, even as an idealization, think of the terms and concepts in a discipline as being defined independently of each other. The ways in which the uses of a term or concept contribute to the epistemic successes of a discipline in practice (and thus the nature of its definition) will depend on the overall inferential architecture and, thus, on the uses and definitions of the other terms in the discipline. This is especially clear in the case of chemistry, even for kinds that do, perhaps, have stereotypical definitions. The practice of chemists since the 1920s of defining elements by atomic number, rather than by atomic mass (and its ratification by

IUPAC in 1923) represented a tacit decision to define elements in terms of the contributions their atoms make to the reactivity of compounds that contain them, with the consequence that the definitions of chemical elements and the structural definitions of compounds are all interrelated via their connection to inferences about reactivity (see, *e.g.*, Paneth 1962, Kragh 2000, Needham 2008, Hendry 2006, 2010). The broader conceptions of kinds and definitions outlined here incorporates such a tacit commitment into a general theory of scientific natural kinds.

We do not deny the importance of natural kinds in the stereotypical sense. If there are kinds in the sciences that fit some version of the stereotypical conception, then they will be important objects of philosophical and scientific study. Perhaps they will be the fundamental kinds in nature.

Nevertheless, we argue, the examples, in synthetic chemistry, of non-stereotypical generalizations framed in terms of non-stereotypical kinds show that an adequate scientific explanation of the epistemic successes of chemists requires that one acknowledge, along the lines just indicated, the role of non-stereotypical natural kind terms and concepts, and of the non-stereotypical natural kinds to which they refer.

Before we explore that theme further, we need to look at a class of chemically important generalizations and chemical kinds that raise issues about natural kind definitions not addressed in the non-stereotypical literature cited above.

3.2 Oxidation states and the problem of conventionality

If the kinds and properties that figure in important non-stereotypical chemical generalizations should be counted as natural kinds in chemistry, then certainly oxidation states will have to be so counted. But the conventionality exhibited by the definition of 'oxidation state' represents a challenge to this idea.

Here is why. Almost all accounts of natural kinds contrast natural kinds with conventionally defined kinds; this is certainly true for accounts that focus on the role of natural kinds in induction and explanation. At least since Locke (1689), philosophers have thought that if chemists relied on purely conventionally defined kinds and categories then their prospects for successful induction would be poor, because there would be no reason for their categorization of substances to align with chemically important properties (see Kornblith 1993, Harré 2005).

What does this have to do with oxidation states? On the one hand, reference to the oxidation states of the atoms in molecules involved in chemical reactions is absolutely central to the ways in which chemists frame their understanding of, and important generalizations about, particular reactions and

classes of reactions. It would thus seem that having some particular oxidation state (say, +2) might be expected to be a natural property in the broader sense under discussion.

On the other hand, the definition of oxidation states is, in a certain sense, about as conventional as any scientific definition can be. The oxidation state of a particular atom in a molecule (or polyatomic ion) is supposed to reflect something about the electron density in its vicinity. The oxidation state of an atom in a molecule is said to correspond to the *hypothetical* charge of that atom, assuming that all the bonds in the molecule are purely ionic. That formulation gets at the idea behind the definition of oxidation state, but it must be carefully understood. It is almost never the case that bonds are, strictly speaking, purely ionic, and, more importantly, there are many cases of covalent bonding where the bonding has very little ionic character. Only in cases where the bonding is mainly ionic does oxidation state closely correspond to electron density. The hypothetical assumption involved in defining the oxidation state of an atom is thus often *deeply* hypothetical: it does not even qualify as ‘hypothetical’ in the usual scientific sense. Instead chemists use *conventional definitions* of ‘oxidation state’ that correspond to the hypothetical formulation where the relevant bonds are mainly ionic, but that deliver determinate values of oxidation state even when the relevant bonds have little or no ionic character.

Let us contrast this ‘hypothetical’ assumption with the assumption involved in methods for calculating approximate molecular energies and wave functions assuming the Born-Oppenheimer approximation. When this approximation is used, the positions of the nuclei in a molecule are treated as fixed parameters, and an approximate solution is sought for the electronic Schrödinger equation of the molecule. One can then systematically vary the fixed parameters of nuclear position (corresponding to the bond lengths and bond angles in the molecule) and calculate approximate electronic energies and wave functions for each, eventually choosing the values of the parameters that minimize the molecule’s total energy. The Born-Oppenheimer approximation is never *exactly* true, but the quantities calculated using it are often very accurate. This is so because, in very many cases, the nuclei move far less quickly than the electrons due to their much greater mass, and thus a highly delocalized electronic wave function, admitting electron motion, is a very good approximation for a given set of nuclear positions. In this sense, the Born-Oppenheimer approximation, while certainly not correct to infinite precision, is vastly less hypothetical, and corresponds much more closely to a physical reality, than the assumptions involved in defining oxidation states.

What is important for our purposes is that the difference in degrees of ‘hypotheticalness’ between the two cases corresponds to a profound difference in the ways in which the hypothetical assumptions are implemented in

practice. In the case of the Born-Oppenheimer approximation, the hypothetical assumption about nuclear motions facilitates answering the theoretical question ‘How are the electron density and energy in a molecule determined?’ by addressing the simpler counterfactual theoretical question ‘How would electron density and energy in a molecule be determined if the position of the nuclei were fixed?’ and by (approximately) solving the Schrödinger equation for an imaginary physical system in which that counterfactual assumption is true. In that regard, it is comparable to any other problem that is made more tractable mathematically by invoking an approximation that ignores a variable that is thought to usually have only a small effect.

The role of the hypothetical assumption in the case of oxidation states is utterly different. For many molecules, it makes theoretical sense to ask what their energy and electron density distribution would be if their nuclei were fixed, and to answer this question by (approximately) solving the electronic Schrödinger equation for such an imaginary system. In contrast, for an overwhelming number of molecules in which bonds are mainly covalent, it makes no theoretical sense whatsoever to ask what the charge density near their constituent nuclei would be if the bonds between them were purely ionic, and to address that question by solving the Schrödinger equation for an imaginary system in which that were so. Instead, chemists assign oxidation states to atoms by applying conventional, formal rules, rather than either physical laws or theoretically justified approximations to those laws. In cases where bonds are mainly covalent, the resulting assignment of oxidation state values to nuclei in atoms is thus only loosely related to the electron density in their vicinity. If, in a reaction, the conventionally defined oxidation state of a particular atom changes from, say, +2 to +1, then this oxidation state change will often, though not always, be concomitant with an increase in the electron density near that atom. (A good example of when this would *not* be the case is when a carbon-carbon double bond in an alkene is hydrogenated: each of the alkene carbon atoms has its oxidation state decrease by one unit, but does not experience a significant increase in electron density, because the electronegativities of hydrogen and carbon are so similar). If, on the other hand, two atoms in different molecules (or even in different regions of the same molecule) share a conventionally defined oxidation state, that fact does *not* reliably indicate that the electron densities near them are significantly similar, especially if the bonds in which they are involved are highly covalent. Indeed, chemists often insist that the definition of oxidation state is ‘conventional’, ‘a formalism’, not actually ‘real’, or something similar.

So, why does the high level of ‘conventionality’ of the way chemists define oxidation states not preclude the methodological and explanatory utility of the oxidation state concept? Why does it not rule out oxidation state as a natural property of an atom in a molecule? A plausible guess, for a non-

chemist, would be that, in practice, chemists use the concept of oxidation state almost exclusively in cases where the relevant bonds are mainly ionic. If this were true, then the Lockean conception that associates conventionality with explanatory and inductive barrenness would be vindicated: in cases where the conventionality in the definition of 'oxidation state' becomes significant, chemists would not use the concept.

The truth is, of course, quite different. Even in many cases where bonding is quite covalent, considerations of oxidation states are still inductively or explanatorily useful. This is so because:

1. With respect to various *particular sorts of reactions*, atoms that are in the same oxidation state, or that can undergo the same change in oxidation state, are often similar in causally and methodologically relevant ways, even though the relevant bonding is mainly covalent.
2. Of course, such methodologically relevant similarities vary from case to case.
3. Chemists, however, know a lot about such cases, even though their knowledge is often (perhaps even typically) partly tacit (and thus non-stereotypical). They have learned, and they teach their students, how to recognize cases in which similarities and differences in oxidation states do matter methodologically, and in what ways they often matter.
4. Thus, even though they may *say* that oxidation states in such cases are purely formal or conventional, chemists' inductive or explanatory uses of the concept of 'oxidation state' are governed by substantive chemical considerations. Chemists do not, for example, assume that there are near universal laws about, say, atoms with an oxidation state of +2. Instead, they rely on partly tacit knowledge of particular sorts of cases in which similarity in oxidation states or in changes in oxidation states do indicate particular sorts of inductively or explanatorily relevant similarities.

These cases include ones where simple approximate rules of thumb involving oxidation states can be useful. For instance, transition metal chemists know that iron often occurs in compounds in the +2 and +3 oxidation states, but rarely +1 or +4. This does not mean that compounds with iron in the +1 or +4 oxidation state cannot be prepared, and it certainly does not mean that their existence would violate a strict physical law. It does, however, suggest that the preparation and isolation of an Fe(I) or Fe(IV) compound would involve significant experimental difficulties to overcome. Sometimes these rules of thumb are more sophisticated than tendency generalizations about which types of compounds are common and which are not. For example, it is a useful tendency generalization that, in most compounds of the lanthanide (lanthanoid) metals (La through Lu), the lanthanide is in the +3 oxidation state. In addition to this tendency generalization, however, it has been noted that compounds with a lanthanide in the +2 oxidation state, such as samari-

um(II) iodide, SmI_2 , are often good single-electron reducing agents, while compounds with a lanthanide in the +4 oxidation state, such as diammonium cerium(IV) nitrate, $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$, are often good single-electron oxidizing agents. This type of generalization is useful when deciding on a reagent necessary for a reduction or oxidation in a synthetic procedure.

Only in very special cases do the useful generalizations involving oxidation states approximate stereotypical generalizations. An example of the latter sort involves compounds with a transition metal in the oxidation state with no valence electrons available for bonding (a so-called d^0 oxidation state). Such compounds strictly *cannot* participate in reactions in which the metal's oxidation state is increased, such as oxidative addition, because such a reaction would involve the energetically prohibitive participation of non-valence ('core') electrons on the metal. Except in cases like this, however, methodologically useful generalizations involving oxidation state perfectly illustrate the points of the present paper.

For cases in which bonding is mainly covalent, and oxidation states are thus largely conventional, oxidation states would *not* function as natural properties if chemists treated them in ways that the stereotypical conception of natural kinds and properties might suggest – if, for example, they looked for 'laws' or high-level generalizations about all, or almost all, atoms in oxidation state +2. Instead, chemists do not, in practice, assume that chemically important categories, properties, or relations (such as oxidation states) must fit the stereotypical conception of natural kinds and properties. The actual inferential architecture of chemistry instead involves deploying chemical categories in highly nuanced ways, informed by local and highly approximate (and partly tacit) non-stereotypical generalizations, as well as by more 'law-like' ones. Instead of anticipating that chemically important categories, properties, or relations will usually be the subjects of something like universal laws, chemists tacitly recognize the role of local and highly approximate (and partly tacit) generalizations as well as the role of more 'law-like' ones.

So, despite the conventionality of their definitions, oxidation states do behave like natural kinds in the broader sense. When the terms and concepts for them are integrated into the rest of the inferential architecture of synthetic chemistry, including explicit and tacit knowledge about particular sorts of reactions, chemists' references to oxidation states do reflect insights about electron density that contribute to their ability to make scientifically informed guesses about reactivity.

3.3 Inferential holism and natural kinds

It might seem, nevertheless, that the way in which chemical insights are reflected in references to oxidation states is strikingly atypical. Atoms in two

different molecules that are each known to have oxidation state +2, say, will not, *simply on the basis of that similarity*, be expected to exhibit important similarities in reactivity. It is only when all sorts of other chemical considerations are brought into play that reference to oxidation states becomes informative.

Is that not very different from the way in which reference to other sorts of natural kinds contributes to the reliability of scientific inferences? Is it not ordinarily to be expected that the similarities that things exhibit *just because they belong to a particular natural kind* will be *by themselves* methodologically important in the relevant discipline?

Probably not. The role of natural kind terms and concepts in chemistry illustrates the important phenomenon of *inferential holism* in science. The definition of a natural kind, on the broader conception, is a matter of the similarities between its various members such that, *given the rest of the inferential architecture of the discipline*, applications of that concept or term allow practitioners to knowledgeably classify relevant phenomena in terms of methodologically relevant similarities and differences. Almost never is it a matter of treating all instances of a kind as relevantly similar in every situation. The kind *compound of chromium* is a natural kind on almost any account of natural kinds, and it almost certainly has a definition meeting the standards set by the stereotypical extrapolation from Putnam's examples. Nevertheless, knowing *just* that a chemical species is a compound of chromium provides a chemist with little useful information about its reactivity. She will need to know (or find out) more about its structure: more about, for example, its oxidation state. It is in the context of the overall inferential architecture of chemistry that knowing that a species is a compound of chromium contributes to making informed guesses about its reactivity.

This is utterly typical of the contribution of natural kinds to scientific understanding. A behavioral ecologist seeking plausible hypotheses about the migration patterns of a particular population of organisms will, of course, need to know what species they belong to, but in most cases she will also need to know much more about its situation: the climate, topography, and biota of the relevant regions. Facts about these factors will, of course, be formulated using a great many other natural kind terms and concepts from behavioral ecology.

Thus, although the extent to which the definition of oxidation states is conventional is initially striking, examination of their role in the inferential architecture of chemistry in fact illustrates an important point about the role of natural kinds in science. Although it makes perfect sense to see the different natural kinds in chemistry (or in any other discipline) as having distinct definitions and inferential roles, the natural kinds in a discipline exhibit their naturalness and manifest their definitions holistically: as components of a

package that includes the concepts, terms, generalizations, inferential practices, instrumentation, research strategies, *etc.* of the discipline.

3.4 Extending the picture: Nonverbal representations

There is an extensive literature on the role of pictorial representations in science, and particularly in chemistry (see, *e.g.*, Hoffmann 2007, Kovac & Weisberg 2011, the papers in Spector & Schummer 2003a/b and the citations therein). We will not attempt to make a contribution to this literature beyond making one proposal.

A final advantage of taking the notion of inferential architecture to be fundamental in understanding scientific representations is that it affords us a way of treating pictures, charts, diagrams, and the like on a par with verbally coded representations. As a simple example, consider the role of ‘arrow-pushing’ diagrams in the formulation of hypotheses about reaction mechanisms, in which the ‘motion’ of a pair of electrons involved in bond breaking or bond formation is represented by a curved arrow, and the motion of a single electron, in reactions involving radical species, is represented by a ‘fish-hook’ curved half-arrow. Such a pictorial notation is used by almost all organic chemists and many inorganic and organometallic chemists. If we think of fully legitimate scientific representations as necessarily verbal entities to which algorithmic rules can apply, we will then have to insist that arrow-pushing diagrams function as legitimate representations of hypotheses about changes in electron density within and between molecules *only* if we assume that, when chemists use those diagrams, they always have in mind a fairly definite ‘translation’ between the diagrams in question and some verbal presentation. Perhaps that is true, but there is no reason to think that the topological and spatial aspects of the hypotheses thus represented, namely, which bond electrons or electron pairs move into or out of, are easily translated. If we move from such simple cases to the representations of protein structures, there is no reason to believe that biochemists even tacitly perform such translations. They might be able to translate the pictorial arrow-pushing representation of the mechanism proposed to operate at an enzyme’s active site. But there is no reason to suppose that they could usefully translate the overall pictorial representation of a macromolecule’s geometry.

More importantly, chemists often do not need to perform even those translations that they could actually accomplish. They do not always need to rely on the sorts of verbally explicit representations highlighted by the stereotypical conceptions. Just as chemists learn their (often discipline-specific) non-stereotypical ways of reading and applying the verbal parts of published papers, they likewise learn (often discipline-specific) ways of looking at and learning from diagrams, charts, pictorial representations, and the like. That

much of what they do (both with verbal and with non-verbal representations) is tacit and non-stereotypical does not diminish the scientific importance of their representations or their inferences. Verbal and non-verbal representations (and their associated inferential practices) are thus scientifically fully on a par with each other.

3.5 One more non-stereotypical factor: Highly social cognitive processes

Scientific work is, of course, a social activity, but the stereotypical conceptions associated with logical empiricism focus on formal aspects of scientific practices, findings, and categories rather than on the social practices involved in scientific research. The non-stereotypical factors explored here obviously involve social practices: they are reflections of the actual inferential architectures of disciplines at a time and are thus of actual social practices in chemistry. Recognizing the social character of inferential architectures permits us to identify an additional feature of scientific reasoning not emphasized by logical empiricism. Although individual scientists do often figure things out by themselves, the good guessing involved in applying *ceteris paratis* (and other) generalizations is often achieved not individualistically, but rather by the sharing of insights in research collaborations – as anyone who has ever participated in meetings of a laboratory research group knows. Similarly, professional conversations at conferences and other sorts of exchanges are, almost certainly, central to the ways in which chemists make *cetera parata* and make conjectures about possible synthetic procedures. When we think of the tacit features of chemists' representations and inferences (and, for that matter, the explicit ones) as part of their discipline's inferential architecture, it is important to remember that not only is the discipline itself a social phenomenon but also, quite often, so is the implementation of its inferential architecture.

4. Making It Explicit?

So deeply entrenched is the stereotypical conception of scientific representations and inferences that one might be inclined to think that the imprecise and partly tacit representations and inferential practices discussed here must somehow be inferior to fully explicit representations and inferential practices. The practice of logical empiricists, and other philosophers influenced by them, of using formal mathematical resources to 'rationally reconstruct' sci-

entific theories and inferential practices using formal mathematical resources lends credibility to that idea.

We will not address here the question of whether, in the fully completed and completely accurate ideal limit of scientific investigations, the sorts of representations we have been discussing would always be inferior to fully explicit ones. We doubt that the question is meaningful, and we are not sure the answer would be 'yes' if it were: perhaps understanding would be enhanced by some less precise, and more tacit, representations and practices.

We will, however, address the question of whether it is, in some way, a failing that chemists have to rely on tacit representations and tacitly understood inferential practices. In a word, no, but there is more to be said. In our view, it is probably almost always a good thing when chemists are able to explicate some of the previously implicit representational or inferential features of their practices, but it is important to recognize just how difficult an achievement that can be. In the first place, even to articulate the dimensions of current tacit practices would be a challenging task. People are not very good at identifying the premises and inferences that underlie their practices: that is why we need philosophers, psychologists, sociologists, and historians of science. But there is a much deeper problem: even such an articulation would not be enough.

Here is why: suppose that someone *were* to make fully explicit the representational and inferential practices characteristic of Lewis structure-type representations of molecular structures, complete with all the patches about 'resonance structures' and the like that prevailed in chemistry before the wide use of different quantum-mechanical approximations such as molecular orbital theory. That would be a major scientific achievement *in cognitive science*. It would probably require the introduction of new concepts and theoretical resources for characterizing inexplicit representation and inferential structures.

It would not, however, be a major scientific achievement *in chemistry*, although it might well contribute to the teaching of beginning chemistry. The sorts of explications that chemists would really value, are ones that make it clearer why, in what respects, and to what extent the Lewis-structure representations represent molecular structures and why, and *to what extent*, the associated inferences are reliable. That is what the introduction of quantum mechanical approximations into descriptions of molecular structures accomplished, *but* that was a major theoretical accomplishment. It was not any kind of failing on the part of earlier chemists that they had not yet worked out molecular orbital conceptions or other quantum mechanical approaches. They had discovered, and usefully (if only approximately) described, the phenomena for which later chemists and physicists offered more detailed theoretical explanations. Likewise, it was not a failing of theoretical chemists

of Pauling's generation, who pioneered many of the applications of quantum mechanics to chemistry, that they did not invent the software and hardware necessary for even more sophisticated contemporary quantum mechanical calculations. Chemists, like all scholars, build on the prior approximate achievements of others.

But might it still be true that, when discoveries or theoretical innovations are made, the advances that clarify features of earlier achievements by scientifically appropriate explication should have pride of place in comparison with other innovations, especially ones that rely on unimproved non-stereotypical representations? We see no reason to think so.

5. Conclusion

Let us sum up, and extract some philosophical lessons.

5.1 How to answer questions about chemical syntheses: How can we synthesize a given compound?

Strategy: Rely on background theories, non-stereotypical generalizations, and tacit conceptions; make, relying on the (partly tacit) *inferential architecture* of the discipline, informed *guesses* about which alternative synthetic techniques are worth considering. Choose between those alternatives using experimental techniques similarly informed by background generalizations, stereotypical and non-stereotypical, deployed *via* the prevailing inferential architecture. Repeat as needed.

5.2 When does this work?

When does it tend to result in approximately correct answers? This strategy works to the extent that:

1. Background representations including tacit and non-linguistic generalizations and non-stereotypical generalizations are true often enough, *ceteris paratis*, and
2. The prevailing inferential architecture, including the resources made available by reference to non-stereotypical natural kinds and properties, is reliable enough *so that*
 - a. Together they underwrite good enough guessing with the results that *often enough* an approximately correct answer is among the resulting guesses *and*
 - b. The experimental techniques they underwrite are, often enough, reliable enough to identify the approximately correct answer.

5.3 Good guessing: In praise of hunches

Here is a less philosophical summary of what we have learned. Good work in synthetic chemistry relies on the ability of chemists to (often enough) make good *guesses* about how to synthesize particular compounds, about what the relevant molecular structures are, and about which reaction mechanisms are operative. They need to be able to reliably generate *hunches* about chemical matters. The hunches they generate, the background chemical knowledge they rely on, the inferential practice that mediate between background knowledge and their hunches, and the kinds, concepts, and other representational machinery they use, often do not fit the stereotypical conceptions, and this is fine for the foreseeable future.

5.4 Is synthetic chemistry atypical?

The special methodological role of guesses and hunches is a scientific universal. In the first place, one cannot test theories or hypotheses that no one has formulated, so guessing (even if one calls it 'hypothesis formation') is essential to science. Much more importantly, when there is progress on scientific questions it is always because, often enough, among the guesses of researchers are some that are relevantly close to the truth (but not necessarily close to the exact *fundamental* truth, whatever that is). That assumption is tacitly built into ordinary standards of evidence: we do not count an hypothesis as well-supported unless it has been tested against other scientifically reasonable guesses (or 'hypotheses,' if one wishes to sound more formal). Standards like this are reliable only when the representational and inferential structures of the relevant disciplines are such that, pretty often some guesses are pretty good (for more and for a discussion of cases where guesses are *not* pretty good, see Boyd 2010).

Still, synthetic chemistry is especially illustrative. Nevertheless, examining synthetic chemistry makes it especially easy to see these points. In the first place, the social character of representations and inferences is especially easy to see. Of course, all science (indeed *all* intellectual inquiry) is social, but the intimacy of the collaboration in synthetic chemistry research groups make it easy to see the extent to which an individual chemist's thinking routinely depends on that of others. This is also true in particle physics, where research groups can have over a hundred members, and sometimes in mathematics, where jointly authored papers are fairly rare, but it is easiest to see in laboratory (bench) sciences like chemistry, where all or most of the participants in a research effort interact, and in those areas of biology involving cooperative field work. In particular, it is easy to see that the implementation of various non-stereotypical representations and inference patterns (and stereotypical

ones too, for that matter) is often mediated by conversations rather than just by individual thinking.

It is likewise important to reflect that one of the pedagogical aims of graduate work in a synthetic chemistry research group is the acquisition of some of the tacit understanding that underwrites non-stereotypical representations and inferences. Of course, something like this is true in every discipline, but the role of research group meetings in graduate education in synthetic chemistry is greater than that in many other disciplines.

It also helps that many of the non-stereotypical representations and inference patterns are widely presented in upper-level undergraduate and graduate level chemistry courses and in textbooks (but typically not in the parts that purport to explain the philosophy of science). Of course, they are usually not made fully explicit (that is the point of this essay), but their role is acknowledged as a regular part of chemical education.

5.5 Representational pluralism

Many historians and philosophers of science have defended broadly pluralist conceptions of scientific representations and practices that criticize aspects of what we have been calling the stereotypical conceptions. We have already mentioned an emphasis on the role of pictorial representations that, we hope, can be assimilated to the framework of inferential architecture that we deploy here. An aspect of this sort of pluralism that is especially relevant to the philosophy of chemistry is the idea that much of the knowledge of synthetic chemists is not the sort of fundamental knowledge celebrated by logical empiricists, and that much of their research is not aimed at testing highly general hypotheses. Instead, much of their knowledge is a matter of know-how: they know how to make new compounds and to experimentally explore particular sorts of chemical reactions. Chang (2012) and Hoffmann (2007) have been especially successful in making these important points about chemical knowledge and practices.

We see the treatment of non-stereotypical representations, inferential practices, and natural kinds offered here as an important complement to Chang's and Hoffmann's emphasis on know-how. Everyone agrees that, in addition to know-how, chemists have lots of 'know-that' knowledge, and that they deploy that knowledge in implementing their know-how. In fact, if one focuses on how synthetic chemists are able to make new compounds and to design particular experiments, it turns out that much of the knowledge that they depend on is represented in non-stereotypical ways and is applied *via* non-stereotypical inferential practices. Thus, the pluralist point that much chemical knowledge is a matter of know-how leads, on reflection, to the pluralist point that much chemical knowledge that is a matter of 'know-

that' involves the rich range of non-stereotypical representational resources described here.

Of course, these points are really quite general with respect to scientific knowledge and practice. What they illustrate is the very non-stereotypical point that an essential feature of science is informed *guessing*.

Three cheers for hunches!

References

- Allred, A.L. & Rochow, E.G.: 1958, 'A scale of electronegativity based on electrostatic force', *Journal of Inorganic and Nuclear Chemistry*, **5**(4), 264–268.
- Ayers, P.W.: 2007, 'The physical basis of the hard/soft acid/base principle', *Faraday Discussions*, **135**, 161–190.
- Beebee, H. & Sabbarton-Leary, N. (eds.): 2010, *The Semantics and Metaphysics of Natural Kinds*, London: Routledge.
- Bhushan, N. & Rosenfeld, S.: 2000, 'Chemical Synthesis: Complexity, Similarity, Natural Kinds, and the Evolution of a 'Logic'', in: N. Bhushan & S. Rosenfeld (eds.), *Of Minds and Molecules*, Oxford: Oxford University Press, pp. 187–210.
- Bhushan, N.: 2006, 'Are Chemical Kinds Natural kinds?', in: D. Baird, E. Scerri & L. McIntyre (eds.), *Philosophy of Chemistry: Synthesis of a New Discipline*, New York: Springer, pp. 327–336.
- Boyd, R.: 2010, 'Realism, Natural Kinds and Philosophical Methods', in: H. Beebee & N. Sabbarton-Leary (eds.), *The Semantics and Metaphysics of Natural Kinds*, London: Routledge, pp. 212–234.
- Chang, H.: 2012, *Is Water H₂O?: Evidence, Realism and Pluralism*, Dordrecht: Springer.
- Christie, M.: 1994, 'Philosophers versus chemists concerning 'laws of nature'', *Studies in History and Philosophy of Science*, **25**, 613–629.
- Christie, M. & Christie, J.R.: 2000, 'Laws' and 'Theories' in Chemistry Do Not Obey the Rules', in: N. Bhushan & S. Rosenfeld (eds.), *Of Minds and Molecules*, Oxford: Oxford University Press, pp. 34–50.
- Christie, J. & Christie, M.: 2003, 'Chemical laws and theories: A response to Vihailem', *Foundations of Chemistry*, **5**(2), 165–174.
- Drago, R.S. & Wayland, B.: 1965, 'A Double-Scale Equation for Correlating Enthalpies of Lewis Acid-Base Interactions', *Journal of the American Chemical Society*, **87**, 3572–3577.
- Evans, D.A.; Bartroli, J.; & Shih, T.L.: 1981, 'Enantioselective Aldol Condensations. 2. Erythro-Selective Chiral Aldol Condensations via Boron Enolates', *Journal of the American Chemical Society*, **103**, 2127–2129.
- Ereshefsky, M & Reydon, T.: 2015, 'Scientific kinds', *Philosophical Studies*, **172**(4), 969–986.
- Griffiths, P.: 1999, 'Squaring the circle: Natural kinds with historical essences', in: R. Wilson (ed.), *Species: New Interdisciplinary Essays*, Cambridge: MIT Press, pp. 209–228.
- Harré, R.: 2005, 'Chemical Kinds and Essences Revisited', *Foundations of Chemistry*, **7**, 7–30.

- Hendry, R.: 2006, 'Elements, Compounds and Other Chemical Kinds', *Philosophy of Science*, **73**, 864-875.
- Hendry, R.: 2010, 'The elements and conceptual change', in H. Beebe & N. Sabbarton-Leary (eds.), *The Semantics and Metaphysics of Natural Kinds*, London: Routledge, pp. 137-158.
- Hoffmann, R.: 2007, 'What might Philosophy of Science Look Like if Chemists had Built it?', *Synthese*, **155**, 321-336.
- Katsuki, T. & Sharpless, K.B.: 1980, 'The First Practical Method for Asymmetric Epoxidation', *Journal of the American Chemical Society*, **102**, 5974-5976.
- Kendig, C. (ed.): 2016, *Natural Kinds and Classification in Scientific Practice*, London & New York: Routledge.
- Kornblith, H.: 1993, *Inductive Inference and Its Natural Ground*, Cambridge, MA: MIT Press.
- Kovac, J. & Weisberg, M.: 2011, *Roald Hoffmann on the Philosophy, Art, and Science of Chemistry*, New York: Oxford University Press.
- Kragh, H.: 2000, 'Conceptual Changes in Chemistry: The Notion of a Chemical Element, ca. 1900-1925', *Studies in History and Philosophy of Modern Physics*, **31B**, 435-450.
- LaPorte, J.: 1996, 'Chemical Kind Term Reference and the Discovery of Essence', *Noûs*, **30**, 112-132.
- LaPorte, J.: 1997, 'Essential Membership', *Philosophy of Science*, **64**, 96-112.
- LaPorte, J.: 2004, *Natural Kinds and Conceptual Change*, Cambridge: Cambridge University Press.
- Locke, J.: 1689, *An Essay Concerning Human Understanding*, London: Thomas Bassett.
- Magnus, P.D.: 2014, 'NK ≠ HPC', *The Philosophical Quarterly*, **64**(256), 387-406.
- Mayr, H.; Breugst, M.; & Ofial, A.R.: 2011, 'Farewell to the HSAB Treatment of Ambident Reactivity', *Angewandte Chemie International Edition*, **50**, 6470-6505.
- Miyaura, N. & Suzuki, A.: 1979, 'Stereoselective Synthesis of Arylated (*E*)-Alkenes by the Reaction of alk-1-enylboranes with Aryl Halides in the Presence of Palladium Catalyst', *Journal of the Chemical Society, Chemical Communications*, **19**, 866-867.
- Mulliken, R.S.: 1934, 'A New Electroaffinity Scale; Together with Data on Valence States and on Valence Ionization Potentials and Electron Affinities', *The Journal of Chemical Physics*, **2**, 782.
- Needham, P.: 2000, 'What is Water?', *Analysis*, **60**, 13-21.
- Needham, P.: 2002, 'The Discovery that Water is H₂O', *International Studies in the Philosophy of Science*, **16**, 205-226.
- Needham, P.: 2008, 'Is Water a Mixture? Bridging the Distinction Between Physical and Chemical Properties', *Studies in History and Philosophy of Science*, **39**, 66-77.
- Paneth, F.A.: 1962, 'The Epistemological Status of the Chemical Concept of Element (II)', *British Journal for the Philosophy of Science*, **13**, 144-160.
- Pauling, L.: 1932, 'The Nature of the Chemical Bond. IV. The Energy of Single Bonds and the Relative Electronegativity of Atoms', *Journal of the American Chemical Society*, **54**(9), 3570-3582.
- Pearson, R.G.: 1963, 'Hard and Soft Acids and Bases', *Journal of the American Chemical Society*, **85**, 3533-3539.
- Psillos, S.: 1999, *Scientific Realism: How Science Tracks Truth*, New York & London: Routledge.

- Putnam, H.: 1975, 'The meaning of 'meaning'', in: H. Putnam, *Mind, Language, and Reality. Collected Papers*, vol. 2, Cambridge: Cambridge University Press, pp. 215-271.
- Slater, M.: 2015, 'Natural Kindness', *The British Journal for the Philosophy of Science*, **66**(2), 375-411.
- Spector, T.I. & Schummer, J. (eds.): 2003a, *Aesthetics and Visualization in Chemistry, Part 1, Hyle: International Journal for Philosophy of Chemistry*, **9**(1), pp. 3-118.
- Spector, T. I. & Schummer J. (eds.): 2003b, *Aesthetics and Visualization in Chemistry, Part 2, Hyle: International Journal for Philosophy of Chemistry*, **9**(2), pp. 129-243.
- van Brakel, J.: 2000, *Philosophy of Chemistry*, Leuven: Leuven University Press.
- van Brakel, J.: 2005, 'On the Inventors of XYZ', *Foundations of Chemistry*, **7**, 57-84.
- van Brakel, J.: 2014, 'Philosophy of Science and Philosophy of Chemistry', *Hyle: International Journal for Philosophy of Chemistry*, **20**(1), 11-57.
- Vihalemm, R.: 2003. 'Are Laws of Nature and Scientific Theories Peculiar in Chemistry? Scrutinizing Mendeleev's Discovery', *Foundations of Chemistry*, **5**(1), 7-22.
- Vihalemm, R.: 2005, 'Chemistry and a Theoretical Model of Science: On the Occasion of a Recent Debate with the Christies', *Foundations of Chemistry*, **7**, 171-182.
- Weisberg, M.: 2006, 'Water is Not H₂O', in: D. Baird, E. Scerri & L. McIntyre (eds.), *Philosophy of Chemistry: Synthesis of a New Discipline*, New York: Springer, pp. 337-345.
- Wilson, R.A.; Barker, M.J. & Brigandt, I.: 2007, 'When Traditional Essentialism Fails: Biological Natural Kinds', *Philosophical Topics*, **35**, 189-215.
- Wilson, R.A.: 1999. 'Realism, Essence, and Kind: Resuscitating Species Essentialism?', in: R. Wilson (ed.), *Species: New Interdisciplinary Essays*, Cambridge: MIT Press, pp. 188-207.

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