

The Metaphysics of Chemistry
First International Workshop
22-24 July 2024
UCLouvain

Programme

Monday 22 July 2024	
08:30	Coffee
09:00	Opening of day 1
09:10	Patric Harting Not All Chemical Kinds Are Natural Kinds <i>Kinds</i> <i>Comments by Emma Tobin</i>
10:00	Micah Newman Explanatory Chemical Kinds <i>Kinds</i> <i>Comments by Luke Miller</i>
10:50	Coffee break
11:10	Marina Paola Banchetti-Robino Boyle and Locke on Natural Kinds <i>Kinds</i> <i>Comments by Alexandre Guay</i>
12:00	Lunch break
13:10	Eric Scerri The Born-Oppenheimer Approximation and the Reduction of Chemistry <i>Reduction</i> <i>Comments by Juan-Camilo Martinez</i>
14:00	Ryan Miller The Irreducibility of Chemistry to Everettian Quantum Mechanics <i>Reduction</i> <i>Comments by Eric Scerri</i>
14:50	Coffee break
15:10	Giorgio Lenta Strong Emergence in Chemistry Entails Counterpossible Non-Vacuity <i>Reduction</i> <i>Comments by Robin Hendry</i>
16:00	Keynote by Emma Tobin Towards A Metaphysics for Biochemical Technologies <i>Reduction</i>
17:30	Closing of day 1

Tuesday 23 July 2024	
08:30	Coffee
09:00	Opening of day 2
09:10	Francesca Bellazzi Vitamins as Investigative Kinds <i>Biochemistry</i> <i>Comments by Charles Pence</i>
10:00	Patrick McGivern Chemical Mechanisms without Reduction <i>Biochemistry</i> <i>Comments by Francesca Bellazzi</i>
10:50	Coffee break
11:10	Pieter Thyssen Disposed to React: A Dispositional Account of Chemical Reactions <i>Causation</i> <i>Comments by Vanessa Seifert</i>
12:00	Lunch break

Tuesday 23 July 2024

13:10	Marabel Riesmeier The Problem of Aromaticity is the Problem of the Chemical Bond <i>Realism</i> <i>Comments by Pieter Thyssen</i>
14:00	Juan-Camilo Martinez Chemists and Philosophers on Acids <i>Realism</i> <i>Comments by Klaus Ruthenberg</i>
14:50	Coffee break
15:10	Vanessa Seifert & James Ladyman Scale Relativity in the Metaphysics of Science <i>Realism</i> <i>Comments by Robin Hendry</i>
16:00	Keynote by Robin Hendry A Pluralist View of Structure and its Role in Classification <i>Realism</i>
17:30	Closing of day 2

Wednesday 24 July 2024

08:30	Coffee
09:00	Opening of day 3
09:10	Klaus Ruthenberg Kant's Metachemistry <i>Realism</i> <i>Comments by Kévin Chalas</i>
10:00	Alan Heiblum Bachelard's Metachemistry <i>Realism</i> <i>Comments by Hannes Van Engeland</i>
10:50	Coffee break and closing of day 3

Presentations will be 25 minutes, followed by a 10 minute commentary by a discussant, a 5 minute reply by the speaker, and a final 10 minutes for Q&A.

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Not All Chemical Kinds Are Natural Kinds

Kinds

Patric Harting (independent)

comments by Emma Tobin

For many defenders of natural kinds the paradigmatic examples are the chemical elements. But the fact that isotopes of the same element have different properties poses a difficulty for this view. I argue that not all chemical kinds are natural kinds, and specifically that isotopes are natural kinds but elements are not.

I develop the view that members of a natural kind must be, in principle, indistinguishable from one another. If proton number is the essence of an element kind, then other properties, such as atomic mass, are accidental and contingent. Accidental, because they are not necessary, and contingent, because they vary with time and place. By contrast, all properties of isotopes, including atomic mass, are necessary and invariant, and this qualifies isotopes as genuine natural kinds.

My view is compatible with microstructural essentialism about natural kinds, which holds that membership of a natural kind is conferred by the microstructural properties of its members. I argue that my view has a number of advantages over other formulations, including views that allow accidental properties, and also over those based on macroscopic properties. This is because my view satisfies the most commonly proposed criteria for natural kind classifications (Bird and Tobin 2023):

- (1) My view provides unambiguous criteria for natural kind membership.
- (2) Natural kinds so understood permit strong inductive inference.
- (3) Natural kinds so understood participate in laws of nature.
- (4) Natural kinds so understood form a natural hierarchy.
- (5) Finally, based on natural kinds so understood we can give a complete and unambiguous description of the world.

Bird, A., Tobin, E. (2023). "Natural Kinds", *The Stanford Encyclopedia of Philosophy* (Spring 2023 Edition). Ed. by E.N. Zalta and U. Nodelman. Available at: <https://plato.stanford.edu/archives/spr2023/entries/natural-kinds/>.

Explanatory Chemical Kinds

Kinds

Micah Newman (independent)

Comments by Luke Miller

Saul Kripke and Hilary Putnam (hereafter KP) argued that nothing could be water if it wasn't H_2O , and nothing could be gold if it was not the element with atomic number 79. Several recent writers have criticized their "microessentialism" along a number of lines. Centrally, they argue that there is no reason to place a priority on microstructure in giving necessary and sufficient conditions for substance identity, and that macroscopic substance terms like "water" itself do not need to be supplemented with any chemical specifications.

There are distinct questions here: (1) Could anything be water without being H_2O ? (Likewise for other substance kinds with purported chemical identities.) (2) Does a chemical essence need to be specified in order to uniquely identify a macroscopic substance? KP answer question (1) with "no" and (2) with "yes." KP's recent critics are concerned with the apparently underlying (2) and arguing for the answer "no," but leave question (1) curiously unaddressed. KP's reasons for answering "no" to (1) have solely to do with their respective versions of semantic externalism, not with anything to do with chemistry. Putnam's "Twin Earth" thought experiment assumes, spuriously, that microstructure could in principle vary independently of macroscopic, "stereotypical" substance properties. It's hard to see this as "microessentialism." I argue that a substantive microessentialist answer "no" should first be given to question (1) because of the ways in which chemical characterizations intimately involve macroscopic properties insofar as they explain them. Furthermore, precisely because of these intimate connections between chemical kinds and macroscopic substance kinds, where "water" (broadly understood) goes, so must H_2O , and vice versa. This microessentialism thus also yields macroessentialism. There is no need to disambiguate between "water" or any sort of impostor like Putnam's "twater" made of "XYZ" because there can be no such thing: the contrastive element of the explanatory basis by which we know chemically how H_2O constitutes water rules out anything that is not H_2O possibly being mistaken for water. So on the same basis just suggested as the answer "no" to (1) was given, (2) can also be answered with "no."

Chemical Taxonomy in Early Modern Science: Boyle and Lock on Natural Kinds

Kinds

Marina Paola Banchetti-Robino (Florida Atlantic University)

Comments by Alexandre Guay

The purpose of this presentation is to situate Robert Boyle both historically and philosophically regarding chemical natural kinds and their taxonomical classification. More specifically, I will compare and contrast the views of Boyle and Locke, precisely because the two men engaged in a lively debate regarding these issues. Although Robert Pasnau argued that Boyle and Locke reached a consensus in favor of taxonomical conventionalism, I will demonstrate that Boyle ultimately favored realism with regards both to chemical kinds and to chemical taxonomy.

The presentation will discuss the points of agreement between Locke and Boyle, such as their mutual rejection of the Aristotelian conception of natural kinds and of the concept of substantial forms. However, it will be argued that Boyle's chemical philosophy leads him to disagree with Locke regarding taxonomical classification and, thus, reject the strictly conventionalist view that chemical classification is purely arbitrary. According to Boyle, since stable chemical concretions have essential form, one can distinguish between those properties of a material body that are accidental and those that are essential, that is, those properties that derive from the stable and operationally irreducible microstructure or essential form of the corpuscular concretions. He also believes, as I will show presently, that it is because of said essential properties that we can establish the species (natural kind) to which a material body belongs.

The Born-Oppenheimer Approximation and the Reduction of Chemistry

Reduction

Eric Scerri (University of California, Los Angeles)

Comments by Juan-Camilo Martinez

The Born-Oppenheimer approximation (BOA) is widely used in theoretical chemistry to solve the Schrödinger equation for any molecule. Several philosophers have claimed that the use of BOA represents a violation of the Heisenberg Uncertainty Principle and that this implies that chemistry does not reduce to quantum mechanics (1,2). These same authors also claim that chemists have no choice but to use BOA in order to solve the appropriate Schrödinger equation for any system. I will argue that both of these claims are mistaken, by examining the nature of the BOA and the more general Born-Huang (B-H) representation (3).

I will provide several arguments to show that the BOA does not in fact imply that the position of nuclei is assumed to be static. One simple objection to the popularly touted view is that the movement of nuclei is more correctly regarded as a small perturbation to the movement of nuclei which is allowed to tend to zero but not to assume a value of zero. The more fundamental objections that I will raise require a more detailed mathematical analysis which draws on the more general framework known as the Born-Huang approach. Similarly, the B-H approach can be used to successfully carry out calculations which go beyond the BOA as will be illustrated with a particular example involving an ultra-fast chemical process.

If the proposal of this paper is correct, it would imply that the often-given reason for the failure of the reduction of chemistry to quantum mechanics would be redundant. Metaphysicians of chemistry would then need to provide completely different reasons if they wish to maintain the failure of the reduction of chemistry, and in particular molecular structure, to quantum mechanics.

(1) H. Chang, Reductionism and the Relation Between Chemistry and Physics, in T. Arabatzis et al (eds), *Relocating the History of Science*, Springer, 2015.

(2) N. Cartwright, *A Philosopher Looks at Science*, Cambridge University Press, 2022.

(3) F. Agostini, B. Curchod, Chemistry without the Born–Oppenheimer approximation, *Trans. R. Soc. A* 380: 20200375. <https://doi.org/10.1098/rsta.2020.0375>

The Irreducibility of Chemistry to Everettian Quantum Mechanics

Reduction | Realism

Ryan Miller (University of Geneva)

Comments by Eric Scerri

The question of whether chemical structure is reducible to Everettian Quantum Mechanics (EQM) should be of interest to philosophers of chemistry and philosophers of physics alike. Among the three realist interpretations of quantum mechanics, EQM resolves the measurement problem by claiming that measurements (now interpreted as instances of decoherence) have indeterminate outcomes absolutely speaking, but determinate outcomes relative to emergent worlds (Maudlin, 1995). Philosophers who wish to be sensitive to the practice of quantum chemistry (e.g. Scerri, 2016) should be interested in EQM because Franklin and Seifert (2020) claim that resolving the measurement problem also resolves the reducibility of chemical structure, and EQM is the interpretation which involves no mathematical structure beyond that used by practicing scientists. Philosophers interested in the quantum interpretation debate should be interested in the reducibility of chemistry because chemical structure is precisely the kind of determinate three-dimensional fact which EQM should be able to ground if it is to be empirically coherent (see Allori, 2023). The prospects for reduction of chemical structure are poor if it cannot succeed in EQM; the prospects for EQM as a guide to ontology are poor if it cannot reduce chemical structure.

Unfortunately for proponents of chemical reduction and EQM, there are three serious barriers to the reduction of chemistry to EQM. The first concern is that quantum treatments of chemical structure rely on the Born-Oppenheimer approximation, which holds nuclear locations fixed while minimizing the energy of the electronic configuration (Hendry, 2022), but this approximation is not licensed by EQM. The Born-Oppenheimer approximation relies on nuclei and molecular orbitals being simultaneously present, but in the three-dimensional ontology following from the Everett interpretation these only emerge at different energy scales and are not simultaneously present (Miller, 2023). The second concern is that the emergent worlds of EQM are supposed to be decoherent at the macro-scale (Wilson, 2020), but the recent development of superchemistry suggests that chemical reactions can occur in coherent states (Zhang et al., 2023). The third concern is that emergent worlds are only pragmatic pseudo-processes (Wallace, 2012), but this means EQM trades realist physics for mere instrumentalism about chemistry.

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Absent a commitment to chemical realism, reduction is an empty promise. The prospects for reduction of chemical structure to EQM are therefore poor.

Strong Emergence in Chemistry Entails Counterpossible Non-Vacuity

Reduction

Giorgia Lenta (University of Genoa)

Comments by Robin Hendry

In a series of papers, Robin Hendry characterizes strong emergence (SE) in chemistry in terms of downward causation. In order to make this precise, Hendry employs a counternomic criterion: claiming that a system exhibits downward causation amounts to claiming «that its behaviour would be different were it determined only by the more basic laws governing the stuff of which it is made (Hendry 2009 p. 185)». In other words, downward causation – and thereby strong emergence – is analyzed in terms of counterfactuals with a physically impossible antecedent. The satisfaction of the counternomic criterion is nicely exemplified by the case of isomers: distinct molecules sharing exactly the same atoms in the same number, but arranged in different structures. For instance, ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) and methoxymethane (CH_3OCH_3), while being composed of the same atoms in the same proportions, display very different properties. This fact is accounted for by their different structures, which are strongly emergent with respect to their lower physical level, at which there are no structural features. In counterfactual terms: «since a molecule's causal powers depend on its structure, its behaviour would be different were it determined by more basic (quantum-mechanical) laws governing the particles of which the molecule is made» (Hendry 2009 p. 189). This seems to provide solid ground for the truth of counterfactuals like the following: (1) if the properties of a molecule were determined at the physical level only, ethanol and methoxymethane would be the same molecule.

Counterfactuals of this kind interact with another thesis endorsed by Hendry (2023): microstructural essentialism (ME), the view that structure is an essential property of substances (qua individual molecules). If molecular structure is strongly emergent, supposing that a molecule's properties are determined at the physical level only amounts to considering a scenario in which molecules have no structure. But if ME is true, this implies that (1) is a counterpossible, namely, a counterfactual with a metaphysically impossible antecedent. Unfortunately, the orthodoxy on counterpossibles (see for instance Williamson 2007) is vacuism: the view that all of them are vacuously true. However, someone who endorses both SE and ME should be unhappy with that: on the

one hand, there is nothing vacuous about the truth of (1), since she could justify it precisely by appealing to the arguments for SE and ME. On the other hand, those same arguments would force her to reject a counterpossible like: (2) if the properties of a molecule were determined at the physical level only, ethanol and methoxymethane would not be the same molecule.

In other words, the combination of SE and ME entails that some counterpossibles are false, contrary to the orthodoxy. In light of this, I aim to further explore the relevant interactions between the metaphysics of chemistry and the formal semantics of counterpossibles, providing a new argument in defense of non-vacuism.

Hendry, Robin F. (2009). "Ontological reduction and molecular structure". In: *Studies in History and Philosophy of Modern Physics*, 41(2010), 183-191.

Hendry, Robin F. (2017). "Prospects for Strong Emergence in Chemistry". In: *Philosophical and Scientific Perspectives on Downward Causation*. Ed. by M. P. Paoletti and F. Orilia. New York: Routledge. 146-163.

Hendry, Robin F. (2023). "Structure, essence and existence in chemistry". In: *Ratio*, 36(4), 274-288.

Williamson, T. (2007). *The Philosophy of Philosophy*. Oxford: Blackwell.

KEYNOTE

Towards a Metaphysics for Biochemical Technologies

Reduction | Biochemistry

Emma Tobin (University College London)

Biochemical approaches to macromolecules are characteristically reductionist, in that they seek to explain biomolecules in terms of underlying chemical processes and structures. Antireductionist accounts are sceptical of reductionist research strategies because they underestimate the biological context and the role of biochemical function. As biomolecules are developed and engineered and as they evolve the clear distinction that we might make between naturally occurring complex macromolecules and those that are the result of biotechnological innovations is difficult to maintain. Emerging biotechnologies often involve man-made or manipulated artefacts designed with a desired biological function. I will use the case of viruses and bacteriophages to explore the distinction between natural phenomena as opposed to biotechnologically designed phenomena such as bacteriophages and MRI vaccines. These cases make the prospects for a purely chemical account of biotechnological molecules look unpromising. I argue that a purely chemical explanations of biological phenomena downplays the contexts of biological phenomena; because the contexts of production, innovation, and evolution in the case of biotechnological artifacts are not properly considered. Biochemical function must play a pivotal role in our metaphysics of biochemical macromolecules.

New Categories Bring Vitality: Vitamins as Investigative Kinds

Kinds | Biochemistry

Francesca Bellazzi (University of Birmingham)

Comments by Charles Pence

Scientific research can be guided by the introduction of new concepts and this can help to develop entire fields of research. Very simply, introducing new categories invites looking for the underlying entities that realise them. However, the question of how to distinguish natural kinds, as categories that capture something independently from how we think of them, from conventions is always open. The situation can get more complicated by cases in which the kinds seem to be half conventional and half natural. In this talk, I will look at the discovery of vitamins B to argue in favour of the notion of investigative kinds, as categories tracking features of the world in a way that shapes fields of research.

I will first present the notions of natural and conventional kinds. Then, I will present the history of the category “vitamin” in nutrition at the end of the 19th century. This history is interesting because the introduction of this category and subsequent scientific discoveries led to the identification of many different vitamins that were originally clustered in various kinds. Specifically, one can notice that the “vitamin B” family is composed of various different macromolecules, which share some properties related to solubility and history, but they differ in terms of the structure and function they have. These differences might indicate the conventionality of the family vitamin B: these molecules are clustered together because of contingent reasons related to their discovery and not based on principles of naturalness. Should we then disregard the category vitamin B, if it does not correspond to a natural kind? I will argue that vitamins can be considered investigative kinds, as those that have to be clarified through empirical inquiry and can lead to further discoveries (Bridgant 2003, Griffiths 2004). Suggesting the existence of the vitamin B family has led to the discovery of real natural kinds, such as vitamin B12 and vitamin B9, and this makes the vitamin category a successful investigative kind. Accordingly, we can retain a notion of investigative kinds that is indeed halfway between conventional and natural.

Bellazzi F. (2022), Biochemical functions, *The British Journal for Philosophy of Science*

Brigandt, I. (2003). Species Pluralism Does Not Imply Species Eliminativism. *Philosophy of Science*, 70(5), 1305-1316.

Griffiths, P. E. (2004). Emotions as Natural and Normative Kinds. *Philosophy of Science*, 71(5), 901–911.

Khalidi, M. A. (2013) *Natural categories and human kinds: Classification in the Natural and Social Sciences*. Cambridge: Cambridge University Press.

Lindblom, K. (2016) The Vitamin B complex. *Report of American Chemical Society*.

Chemical Mechanisms Without Reduction – A Case Study from Biochemistry

Reduction | Biochemistry

Patrick McGivern (University of Wollongong)

Comments by Francesca Bellazzi

The aim of this paper is to consider the relationship between chemistry and other sciences by examining the metaphysical significance of biochemical mechanisms in simple living systems. While many discussions of reductionism, emergentism etc. in the metaphysics of chemistry focus on the reducibility of chemistry to physics, the focus here is on the significance of chemical mechanisms for our understanding of processes and phenomena in other sciences – in particular, the life sciences. Does the identification of (bio)-chemical mechanisms necessarily lead to a form of reduction?

My approach to this question begins with Hendry's recent anti-reductionist account of chemical mechanisms (Hendry 2023). Hendry argues that mechanisms are central to chemistry and that chemical mechanisms fundamentally involve “the breaking of making of bonds between atoms”. Yet he also argues that this view doesn't lead to the reduction of chemical phenomena, since “the ‘lower-level’ entities can do what they do [viz. make and break bonds] only when embedded in higher-level organisation or structure.”. In this paper, I try to apply a similar line of reasoning to cases involving biochemical mechanisms, asking what sorts of higher-level organisation or structures would be necessary in specific cases in order to undermine reduction in the manner Hendry suggests.

A key set of examples comes from recent work at the intersection of biology and the cognitive sciences. Here, much recent work focuses on ‘minimal’ or ‘basal’ forms of agency found in single-celled organisms, such as bacteria (Lyon et al 2021). Two forms of bacterial behavior have received particular attention: bacterial chemotaxis (where individual bacteria are able to selectively follow chemical gradients in their environments, supposedly demonstrating a minimal capacity for selective action) and quorum sensing (where groups of bacteria are able to engage in minimal forms of communication, and subsequently alter their behavior once a particular threshold condition is satisfied). In both cases, there has been much research on the underlying biochemical mechanisms responsible for these behaviors. In many cases, the underlying biochemical mechanisms have been described in significant detail. What remains unclear is what the metaphysical significance of these biochemical mechanisms is. Some philosophers appear to endorse

what I will call the principle of ‘mechanistic exclusion’, whereby the presence of a biochemical mechanism – and the availability of a biochemical mechanistic explanation – excludes the need for any higher-level explanation (in terms of agency, goal-directed action, or any similar concepts from the life sciences), except as a matter of pragmatic convenience (Adams 2018). Against this, I will argue that these higher-level concepts are compatible with a mechanistic basis: the underlying mechanisms allow us to understand how these capacities are realised in specific contexts, but these mechanisms can only be fully understood within the broad context of the higher-level structures they are parts of.

Adams, F., 2018. Cognition wars. *Studies in History and Philosophy of Science Part A*, 68, pp.20-30.

Hendry, R.F., 2023. Mechanisms in Chemistry. In *New Mechanism: Explanation, Emergence and Reduction* (pp. 139-160). Cham: Springer International Publishing.

Lyon P, Keijzer F, Arendt D, Levin M., 2021 Reframing cognition: getting down to biological basics. *Phil. Trans. R. Soc. B* 376: 20190750.

Disposed to React: A Dispositional Account of Chemical Reactions

Causation

Pieter Thyssen (UCLouvain)

Comments by Vanessa Seifert

The **nature of chemical causation** has seldom been discussed. To wit, in the entire 747-page *Oxford Handbook of Causation*, the word ‘chemistry’ appears only once! And yet, chemistry is replete with causal talk. **Chemical reactions**, in particular, are paradigmatic examples of *causal processes* in which one set of chemical species (the *reactants*) is converted into another set of chemical species (the *products*).

While Goodwin [1] and Hendry [2] have hinted at the possibility that chemical reactions may involve a **conserved-quantity conception of causation**, neither has developed this line of thought. Statham [3] and Ramsey [4], in contrast, have applied Woodward’s **interventionist theory of causation** to chemical reactions, albeit with varying success. All of this begs the question whether chemical reactions are susceptible to causal analysis, and if so, which account of causation best applies to them.

The aim of this talk is to offer a **dispositionalist analysis of chemical causation**. The idea is that the properties of chemical kinds *qua* dispositional powers *bring about* certain chemical reactions when triggered by the right chemical environment. Brønsted acids, for example, have the *disposition* to donate a proton when put into contact with a base. This *brings about* a proton transfer between the acid and base, which chemists identify as a neutralisation reaction. I will attempt to develop this idea within the framework of **causal dispositionalism** [5]. I will thus reject the overly simplistic trigger–manifestation model of how causal powers are activated, and rely instead on the notion of **mutual manifestation**. On this account, “causation occurs when two or more reciprocal disposition partners come together to produce a mutual manifestation” [6].

I will argue that this account is particularly apt to describe the **causal nature of chemical reactions**. Indeed, while an acid only manifests its acidity (by donating a proton) when a base is present (to accept the proton), a base only manifests its basicity in the presence of an acid. As such, it is difficult to tell what is trigger, and what is manifestation. Rather than picturing it in such asymmetric terms, the mutual manifestation account emphasises the *symmetry*—the mutuality—of the causal change [6]. A neutralisation reaction, on this view, does not consist of the active power of an acid working on a passive base, or vice versa. Rather, both the acid and base have chemical dispositions that

interact with one another, so as to mutually manifest the production of an ionic salt and water.

Building on a distinction drawn by Baltimore [7], I will compare and defend the mutual manifestation view against the closely related, but importantly different, **contribution combination view** of causation, and briefly discuss whether the mutual manifestation view can be extended to *all* chemical reactions.

[1] Goodwin, W. (2012). “Mechanisms and Chemical Reaction.” In: *Handbook of the Philosophy of Science: Philosophy of Chemistry*. Ed. by A. I. Woody, R. F. Hendry, and P. Needham. Amsterdam: Elsevier.

[2] Hendry, R. F. (2017). “Mechanisms and Reduction in Organic Chemistry.” In: *EPSA15 Selected Papers*. Ed. by Massimi, M. et al. European Studies in Philosophy of Science.

[3] Statham, G. (2017). “The Manipulation of Chemical Reactions: Probing the Limits of Interventionism.” In: *Synthese*, 194, 4815–4838.

[4] Ramsey, J. L. (2008). “Mechanisms and Their Explanatory Challenges in Organic Chemistry.” In: *Philosophy of Science*, 75, 970–982.

[5] Martin, C. B. (2008). *The Mind in Nature*. Oxford: Oxford University Press.

[6] Mumford, M., Anjum, R. L. (2018). “Dispositionalism: A Dynamic Theory of Causation.” In: *Everything Flows: Towards a Processual Philosophy of Biology*. Ed. by D. J. Nicholson and J. Dupré. Oxford: Oxford University Press.

[7] Baltimore, J. A. (2022). “Dispositionalism, Causation, and the Interaction Gap.” In: *Erkenntnis* 87, 677–692.

The Problem of Aromaticity is the Problem of the Chemical Bond

Kinds | Realism

Marabel Riesmeier (University of Cambridge)

Comments by Pieter Thyssen

Aromaticity plays a crucial role in understanding molecular structure, reactivity, and material properties of many organic and inorganic compounds. Initially describing special properties in certain planar organic ring structures, the concept has been expanded and applied to a diverse range of molecules. Yet, there is considerable disagreement about the definition of aromaticity. Even IUPAC does not give a unique definition but lists a range of criteria that generally characterise aromaticity, but may diverge in practical cases. The conceptual disagreements are serious concerns to practicing chemists, some of whom diagnose a crisis in the field of aromaticity research (Merino et al. 2023).

In this paper, I argue that the problem facing the aromaticity research community today has considerable parallels in debates on the chemical bond among philosophers of chemistry. Just like bonds (Hendry 2008), aromaticity can either be viewed as something structural that has some material equivalent, or something energetic, a way of bonding. Commonly used candidate criteria of aromaticity, such as ring currents, structural data, and resonance energy can be mapped onto this distinction. I connect these debates to practical concerns of observable vs. unobservable properties in aromaticity research. It is interesting to note that the ambiguities in the definition of the chemical bond are rarely seen as a threat to chemical practice, yet a very similar problem is seen as a serious crisis in the case of aromaticity.

Aromaticity is sometimes considered a (very successful) model. I argue that this view is mistaken. Aromaticity describes a phenomenon that can be modelled and measured in multiple ways. Models of aromaticity are useful ways of drawing precise boundaries around the phenomenon in a binary way, but ultimately describe an interactive property that is not binary and only emerges in the relationship between a molecule's constituents. I argue that aromaticity can be understood as a real pattern analogous to Seifert (2023) and explore the implications of this move. Considering aromaticity a real pattern has the advantage of circumventing the calls for an underlying or unifying definition, but it does not settle the question of aromaticity in boundary cases. I argue that such boundary cases may be of practical concern in research politics, but do not threaten the stability

of aromaticity as a phenomenon. Identifying aromaticity with one model, no matter which side of Hendry's (2008) distinction, may settle edge cases but ultimately risks losing sight of the nuanced reality of the phenomenon.

Hendry, R. F. (2008). Two Conceptions of the Chemical Bond. *Philosophy of Science*, 75(5), 909–920.

Merino, G., Solà, M., Fernández, I., Foroutan-Nejad, C., Lazzeretti, P., Frenking, G., Anderson, H. L., Sundholm, D., Cossío, F. P., Petrukhina, M. A., Wu, J., Wu, J. I., & Restrepo, A. (2023). Aromaticity: Quo Vadis. *Chemical Science*, 14(21), 5569–5576.

Seifert, V. A. (2023). The Chemical Bond is a Real Pattern. *Philosophy of Science*, 90(2), 269–287.

Chemists and Philosophers on Acids

Kinds | Realism

Juan-Camilo Martinez (University of Buenos Aires)

Comments by Klaus Ruthenberg

A recent debate regarding the class of substances known as acids has emphasized the different models that classify them. In particular, the debate revolves around the possibility that the Arrhenius and Brønsted-Lowry models are special cases of G.N. Lewis's model (Scerri 2022), and that this, in turn, is a particular case of the Sanderson Mulliken model of covalent bonds or Molecular Orbital (MO). Tantillo and Seeman (2023) attempt “to respond to several publications in the philosophy of science literature that have suggested the lack of a unified theory of acidity (Tantillo and Seeman 2023), in their article, detailing the explanation of the acid-base pair in terms of MO.

This article discusses two aspects regarding acids: is there a divergence concerning the Brønsted-Lowry and G.N. Lewis acids? In favor of Chang (2012) and Ruthenberg and Chang (2017), the divergence exists: the way acidity is measured in both models differs. While there is a pH meter for Arrhenius and Brønsted-Lowry acids, in Lewis model (Scerri 2022) and the HOMO/LUMO only the strength of an acid can be determined, and various indirect methods can be used for this purpose. On the other hand, the divergence could be coincided in terms of the dependence of these models on specific theories; the three models belong to different theoretical moments in the historical development of physical chemistry. From the ionists Arrhenius, Ostwald, and van't Hoff to the introduction of approaches to apply Gibbs' thermodynamics by Lewis, to the development of the molecular orbital model in the realm of quantum chemistry. This divergence highlights that chemical properties are model-dependent, something that has gained traction in the field of philosophy of measurement, in the so-called modelbased account of measurement. In Chang (2012) and Ruthenberg and Chang (2017), there is an epistemic priority regarding the materiality of the model used for measurement, such as the pH meter, while in Scerri and Tantillo Seeman, models of other typologies fulfill the role of measurement instruments. Although this idea has been suggested in Morrison (2009), paying attention to the case of measuring certain chemical properties can help consider a typology of models that serve measurement functions.

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Scale Relativity in the Metaphysics of Science

Kinds | Causation | Realism

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James Ladyman (University of Bristol)

Comments by Robin Hendry

We formulate three novel arguments for the importance of scale-relativity in the metaphysics of chemistry, further supporting the general idea of scale-relative ontology (Ladyman and Ross 2007). We consider chemical substances, elements, and catalysts, and show that in all three cases consideration of scale is vital in order to make claims about natural kindhood, realism and causation respectively.

First, chemical substances are by definition entities that are in thermodynamic equilibrium. That is, chemists identify substances as such when they are thermodynamically stable. The International Union for Pure and Applied Chemistry states that a chemical species is stable always with respect to “some explicitly stated or implicitly assumed standard” (and with respect to a particular transformation; IUPAC 2014: 1432). The standard corresponds to the thermodynamic values that are “characterized by a standard pressure, molality or amount concentration” (IUPAC 2014: 1438). Therefore, stability is a scale-relative property and being admitted as a chemical substance is scale-relative. This in turn affects whether substances can be understood as natural kinds as it is often required that kinds are unified by a natural property. If the fact that stability is scale-relative implies it is not a natural property, the claim that substances are natural kinds would be undermined. This kind of scale-relativity also has implications for different forms of realism about chemical substances. A similar point is made by Hendry who, in support of his emergentist view, argues that a substance’s existence and structure are both “scale-dependent” (2021: 44). However, whether scale-relativity requires strong emergence, or is compatible with physicalism or reductionism are matters for further analysis.

Questions about the reality of chemical elements also involve scale. In the past, chemical elements were discovered under normal thermodynamic conditions, and were empirically observable in macroscopic quantities and for amounts of time measured in seconds if much longer. Recent work on superheavy elements shows that this is no longer empirically possible. Scientists have now drastically reduced the range of time required to accept the discovery of an element: “(d)iscovery of a chemical element is the experimental demonstration, beyond reasonable doubt, of the existence of a nuclide with an atomic number Z not identified before, existing for at least 10-14 s” (Wapstra

1991: 883). This implies that the admittance of new elements into our ontology (as represented by the periodic table) is a scale-relative matter.

Finally, while catalysts are often vital for the realisation of a chemical reaction, they are not admitted as reactants as they do not chemically transform into any of the relevant products. However, the study of reaction mechanisms shows that there are intermediary stages in a reaction during which catalysts chemically transform before taking back their initial form. This suggests that considering catalysts as background conditions instead of reactants is a scale-relative matter. This is relevant to how chemical reactions are understood causally, since a catalyst may be neither necessary nor sufficient for a reaction to take place, while being part of a component causal process.

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KEYNOTE

Islands of Order: A Pluralist View of Structure and its Role in Classification

Realism

Robin Hendry (Durham University)

In this paper I present a pluralist conception of structure at the molecular scale, and its role in classification in the physical sciences. Drawing on examples from chemistry, condensed matter physics and crystallography, I argue that structural theories embody distinct sets of iterative rules for generating composite objects from a stock of more basic items. However, the rules governing composition have finite areas of application because they make substantive physical and metaphysical assumptions about how the materials they describe are constructed. Where these assumptions break down, different theories of structure are needed. One might say that structural theories describe islands of order in seas of disorder.

1. Crystal structures are classically understood as being generated by repetitions of unit cells composed of discrete atoms, ions or molecules. In one sense the breakdown of order is concrete and prosaic: these neat arrays are disrupted by the application of heat. At around 800°C for instance, the regular structure of sodium chloride breaks down when enough of the sodium and chloride ions acquire enough energy to escape the forces holding them together, forming a liquid consisting mostly of dissociated ions. On a less prosaic note, the classical idea of structure is idealised, and embodies non-trivial assumptions about composition, and the composite objects so formed. Even in the solid state, impurities and defects disrupt the regularity of real crystal lattices, and their presence is key to understanding many properties of solid materials. Moreover, classical conceptions of crystal structure make a tacit assumption of translational symmetry, which comes with the idea of repeated unit cells: a form of 3-dimensional tessellation. Dan Shechtman's discovery of quasi-crystals, for which he was awarded the 2011 Nobel Prize in Chemistry, showed that some materials have crystal-like structures that violate this assumption.
2. The familiar structural formulae of organic chemistry are generated by a theory that emerged in the 1860s, to account for the existence of the many cases of isomerism in compounds containing carbon, hydrogen, nitrogen and oxygen. The structures it generates are quite distinct from those attributed to crystals, being built up from

pairwise bonds between atoms, rather than geometrical relationships between them. The theory was refined over the ensuing decades in the light of new chemical discoveries, and emerging experimental methods such as X-ray crystallography and infrared spectroscopy. It was known from the outset that the rules of valence generating these classical structures do not hold in every compound. Multiple anomalies were known within organic chemistry, and Alfred Werner was awarded the 1913 Nobel Prize in Chemistry for his work on the structure of coordination compounds which, he argued, violated the rules of valence. The application of quantum mechanics has deepened and qualified the classical conception of valence structure in many ways, but it has not yet replaced it.

It is a distinctive (though not unique) feature of this pluralism that it is motivated by the subject matter of structural theories, rather than the interests of those who study it.

Kant's Metachemistry

Kinds | Realism

Klaus Ruthenberg (Courg University of Applied Sciences and Arts)

Comments by Kévin Chalas

Although his philosophy of science was strongly influenced by Newton's physics, Immanuel Kant can be considered the first modern philosopher to explicitly address chemistry. An important part of his supposedly stern verdict from 1786 that chemistry cannot become a "proper science" is usually neglected in recent discussions in the history and philosophy of chemistry – the denotation as systematic art. Although the final truth about the "world-in-itself" is inaccessible according to Kant, he admits empirically driven scientific progress, which can be clearly documented by his references to theoretical attempts – first Stahl, then Lavoisier. In fact, chemistry is – even today – a systematic art. The present paper tries to flesh out this claim using, along with Kant's own works, the commentaries of two critical chemist-philosophers, Hans Cornelius and Friedrich Paneth.

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Bachelard's Metachemistry

Realism

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Comments by Hannes Van Engeland

In his philosophy of science (1928-1972), Bachelard embraced the Kantian system with a notable exception, challenging the notion that the conscious mind is fixed and universal. A compelling departure from this perspective is evident in his introduction of the intriguing term Metachemistry. On the one hand, it can be said that Physics is a science of being; correspondingly, Metaphysics is about conditions of possibility. On the other, Chemistry is a science of becoming; correspondingly, Metachemistry is about conditions of combinability. While the concept of Metachemistry was extensively developed in *The Philosophy of Non* (1936), it is less known that its initial appearance dates back to 1932 in *The Coherent Pluralism of Modern Chemistry*. In this work, I explore the reasons behind Bachelard's statement that elucidating the correlative character notions of chemistry, was the true task of a Chemical Philosophy.

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