

Natural kinds and topics in the philosophy of chemistry

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 - Natural kinds are not a priori

- 2 Two views of chemical substances
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 - Macroscopic conceptions of substance

Topics in the philosophy of chemistry



Michael Weisberg, Paul Needham, and Robin Hendry (2019). *Philosophy of chemistry*. In Edward N. Zalta (ed.), *Stanford Encyclopedia of Philosophy*, <https://plato.stanford.edu/entries/chemistry/>.

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Chemical reduction



Michael Weisberg, Paul Needham, and Robin Hendry (2019). *Philosophy of chemistry*. In Edward N. Zalta (ed.), *Stanford Encyclopedia of Philosophy*, <https://plato.stanford.edu/entries/chemistry/>.

- Common belief (among chemists and philosophers alike): chemistry is reducible to physics
- But philosophers of chemistry are often sceptical of this possibility. Let's distinguish two questions:

Question

Are atomic and molecular species reducible to systems of fundamental particles interacting according to quantum mechanics?

Question

Are (macroscopically described) chemical substances reducible to (microscopically described) molecular species?

Reduction of molecular species to quantum physics

Often considered relatively unproblematic, there are in fact severe obstacles to such a reduction:

- Chemical concepts such as valence and bonding, as well as molecular shape, are hard to account for in quantum physics.
 - The errors introduced in approximations (such as strong idealisations) in quantum-mechanical calculations of chemical properties cannot be estimated.
 - The **length of periods** in the periodic table cannot be derived from quantum physics without experimentally determined chemical information is added.
- ⇒ At least so far, **chemistry has not been reduced to quantum physics**—whether it's in principle possible remains open.

Reduction of substances to molecular species

Again, this reduction is often assumed to be unproblematic, but philosophers of chemistry have urged caution:

- A reduction of temperature to microscopic conditions for a gas temperature are circular.
- Much harder cases for reduction of macro to micro: phase transitions, chemical properties such as solubility and reactivity, etc.

Weisberg, Needham, Hendry (2019, §6.2):

While there is no in-principle argument that reductions will always be impossible, essential reference is made back to some macroscopically observable chemical property in every formal attempt of reduction that we are aware of. In the absence of definite arguments to the contrary, it seems reasonable to suppose that chemistry employs both macroscopic and microscopic concepts in detailed theories which it strives to integrate into a unified view.

Natural kinds and chemical kinds



Robin Findlay Hendry (2016). Natural kinds in chemistry. In Eric Scerri and Grant Fisher (eds.), *Essays in the Philosophy of Chemistry*, Oxford University Press: New York, 253-275.

Thesis (Hendry)

A priori requirements for natural kinds, such as that they must be hierarchical, discrete, and independent of interests, are undermined by chemistry.

- Hendry: there are various ways of individuating 'substances'—in chemistry, it's done at the **level of microstructures**.
- For two reasons:
 - 1 This captures the interest-dependent classificatory practices in chemistry; and
 - 2 macroscopic individuation fails.
- causal argument for **microstructural essentialism**

Thesis (Hendry)

Chemical kinds are natural kinds.

Chemical kinds

Hendry (2016, 253):

Chemistry is in the business of making general claims about substances, a fact which is embodied in the periodic table, as well as in the system of nomenclature and classification published by the International Union of Pure and Applied Chemistry (IUPAC).

- main kinds of chemical kinds: chemical substances (gold, water, benzene) and microstructural species (gold atoms, water and benzene molecules)
- higher kinds of substances: **groups of elements**, such as halogens and alkali metals, or even broader groups of elements, such as metals, and **classes of compounds** either sharing an elemental component (e.g., chlorides), a microstructural feature (e.g., carboxylic acids), or a pattern of chemical reactivity (e.g., acids)

Substances vs microstructural species

Careful with chemical formulae:

They may name both substances and microstructural species. For example, 'H₂O' names both a molecular species (an oxygen atom bounded to two hydrogen atoms), as well as a substance composed of hydrogen and oxygen in the molecular ratio 2:1.

- Conceptually, we need to distinguish the two...
- Not every micro-species corresponds to substance:
 - Some correspond only to parts of substances (Ex: H₃O⁺, NH₄⁺).
 - Some are too short-lived to correspond to stable substance (Ex: He₂), even though they may be explanatorily important (Ex: carbonium ions)
- Not every substance corresponds to a single micro-species:
 - Salt contains sodium (Na⁺) and chloride (Cl⁻) ions in a lattice.
 - Another example: water

Metal, silk, wood, and food...

- different scientific disciplines or craft practices use terms differently: e.g. astronomers only distinguish hydrogen and helium, all other elements are 'metals'
 - Example: chemically identical, but artificial 'silk' is not considered silk because it has not been produced by silkworm (which produces silk which may be chemically heterogeneous, as it may depend on environmental factors)
- ⇒ causal history of substance may be more important than chemical composition
- Same goes for wood, wool, foodstuffs.
 - Example: 'jade' names two chemically distinct substances, jadeite and nephrite
- ⇒ appearance (and economics!) may be as important as constitution

However, the relevance of these non-compositional factors (causal history, appearance) derives from classificatory interests foreign to chemistry, even though they may of course have just as much a claim to objectivity as chemical classification. Let's focus on chemistry.

What are natural kinds?

Question:

What makes a scientific category a natural kind?

- natural occurrence vs natural groupings of entities: mostly concerned with second
- notion of chemical substance emerges when chemists start to use 'affinity tables': substances are composed of 'building blocks' which persist through chemical change (module on history of chemistry)
- 'natural': best understood in opposition to 'arbitrary', not 'artificial'
- How do we identify natural kinds?
- We could set up necessary conditions, in a priori way...

Hendry (2016, 257)

[I]f the requirements are chosen poorly, then virtually no chemical kinds will count as natural. In what follows I will consider and reject three such a priori requirements: (i) hierarchy (there can be no overlap between two kinds unless one contains the other); (ii) discreteness, and (iii) independence from interests.

(i) Hierarchy

Condition (Hierarchy)

No two natural kinds may overlap unless one includes the other, or both are included within a third.

- motivation: natural kinds should form single system

Counterexample

There is an overlap between tin and metals, but neither encompasses the other: tin comes in two forms, 'white' (metallic) and 'gray' (non-metallic), and can transform from one form to the other (tin pest).

- Reply: could challenge either of these as natural kinds, but...
 - **Tin** is an element (Sn, atomic number 50), with characteristic chemical and physical behaviour.
 - **Metals** have particular structure of array of ions with many relatively free electrons, which explains e.g. electrical and thermal conductivity.
- ⇒ **Reply unconvincing**, and difficult to see how condition could be weakened without making it vacuous.

(ii) Discreteness

Condition (Discreteness)

Natural kinds must be discrete, i.e., it must consist in divisions (Plato's metaphor of "cutting nature at its joints").

Ellis (2002, 26)

*The elements and their various compounds are all **categorically distinct** from each other [...] in the sense that there is never a gradual transition from any one chemical kinds to any other chemical kind [...] Where there are such [continuous] transitions in nature, as there are between the colours, for example, we have to draw a line somewhere if we wish to make a distinction.*

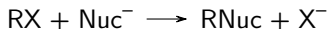
Thesis (Hendry)

Continuous transformations between two chemical kinds do not mean that they are not objectively distinct. Furthermore, chemical variety is continuous—except for the elements.

(ii) Discreteness

Three arguments for Hendry's thesis:

- 1 Chemical kinds are individuated by their microstructures, and the microstructures of compound substances are defined by **continuously varying quantities** such as distances between atoms.
- 2 Such continuous transitions between distinct chemical species is how **chemical change** takes place. For example, a reaction of an alkyl halide RX (such as bromoethane) with nucleophilic ion Nuc⁻ (e.g. hydroxyl ion OH⁻):



can be considered continuous, even though it involves a breaking of a bond between the halogen atom and the neighbouring carbon atom in the alkyl group.

- 3 Chemical change from one stable substance to another involves gradual journey through across **continuous potential energy surfaces**, so chemical kinds are not discrete.

(iii) Independence of interests

Condition (Independence of interests)

Natural kinds are independent of the interests of classifiers.

Thesis (Hendry)

*“While the **existence** of classes of atoms like nuclear charge (or of atomic weight) is clearly not interest-dependent, chemists’ focus on nuclear charge rather than atomic weight clearly is. I [...] do not think that this in any way undermines their status as natural kinds.” (2016, 261)*

- focus on nuclear charge (rather than atomic weight) is a choice, because it is main determinant of chemical behaviour (consider isotopically diverse substances such as silver, mercury, and tin)
- structure (and therefore chemical classification) is interest-dependent: there are different structures—bond structure, geometric structure, etc—none of which is more fundamental, but they are objective

Summary

- All three a priori requirements for what it is to be a natural kind fail for chemical kinds.
- But: chemical kinds are prototypical of natural kinds, and so we need a different approach to what a natural kind is.
- Naturalist approach: natural kinds are based on genuine similarities and differences that underwrite scientific understanding

Hendry (2016, 262)

*[T]he weak realist view is that a kind is natural insofar as its members share some property which is causally relevant to maintaining the regularities in behavior whose existence underlies the very usefulness of the notion of a natural kind [...]. The formation of classificatory **systems** is undeniably an important part of science [...], but it is something that arises as a feature of highly developed explanatory systems. It cannot be imposed a priori.*

Two views of chemical substances

Main question:

Given that chemistry deals with both substances—macroscopic bodies of stuff—and the molecular species they are constituted by, how are substances and molecular species related to one another?

Position (Microstructuralism)

Chemical substances are individuated in terms of their characteristic molecular constituents.

Position (Macroscopic conception of substance)

Substances are individuated by their macroscopic behaviour and properties (rather than by their microstructures).

Microscopic conceptions of substance

Three arguments in favour of microstructuralism

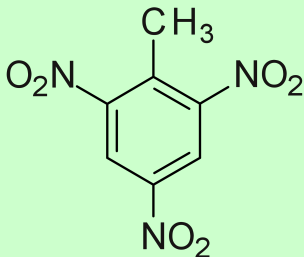
- Hendry gives three discipline-specific arguments in favour of microstructuralism which are grounded in the theories, practices, and interests of chemistry itself, rather than being metaphysical a priori arguments.

First argument: nomenclature

Argument

"[M]icrostructure is the basis of chemistry's own classification of, and nomenclature for, chemical substances." (Hendry 2016, 264)

Example: 2 4 6-trinitrotobulene (TNT)



- basis is **tobulene** (or 'methylbenzene'): six carbon atoms bound in benzene ring with a methyl (-CH₃) group attached
 - **trinitrotobulene** because it contains three substituent nitro (NO₂) groups
 - **2 4 6-trinitrotobulene** because these three groups are placed at second, fourth, and sixth places counting from the methyl group as 1
- The IUPAC has defined systematic ways of naming chemical substances, referring exclusively to microstructural features.

Second argument: explanation

Argument

"[M]icrostructural properties and relations are involved indispensably in explanations of the physical properties, chemical reactivity, and spectroscopic behavior of chemical substances." (Hendry 2016, 264)

- **physical properties:** e.g. boiling point depends on strength of intermolecular forces required to free molecules from liquid, which depends on size and structure of atoms and charge distribution
- **chemical reactivity:** reaction mechanism begins and ends with structure, going through structural changes
- **spectroscopy:** absorption or emission of light is understood via interaction of specific parts of molecule with light of relevant wavelength

Third argument: no alternative

Argument

"[T]here is no alternative. There is no conception of the sameness and difference of chemical substances that is both independent of microstructure and consistent with the ways in which chemistry in fact classifies substances, and how it explains their behavior." (Hendry 2016, 265)

- This pretty much establishes microstructuralism.
- "Pretty much", because there are pairs of macroscopically distinct substances which are pretty much the same microscopically

Example: red and yellow mercury chloride

- Both consist of same repeating units (-O-Hg-O-), but differ in colour and size of lumps into which they are aggregated.
- Difference results from difference in process how substance was formed.
- However, lump size is also a microstructural difference.

Objection to microstructuralism: heterogeneity

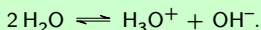
Objection

"[E]lements and compounds can be heterogeneous at the microstructural level." (Hendry 2016, 266)

Example: water

Liquid water is not homogeneous at the molecular level:

- Some H₂O molecules dissociate, forming H₃O⁺ and OH⁻ ions:



- Importantly, these ionic dissociation products are not 'impurities', as their presence is central in explaining water's electrical conductivity.
- Moreover, H₂O molecules form hydrogen-bonded chains.

- But molecular heterogeneity is consistent with microstructuralism, water is not assemblage of H₂O molecules, but "heterogeneous molecular population that is generated by bringing H₂O molecules together" (ibid)

⇒ Microstructuralism is not the view that substances are homogeneous populations of molecular or atomic species, but instead only requires that populations as a whole have some characteristic microstructural property.

Macroscopic conceptions of substance

(1) Substances are nodes in productive networks

Hendry (2016, 269):

[A]ccording to van Brakel (2000, Chapter 3), chemistry is a “science of stuffs” that manipulates and transforms macroscopic quantities of substances, investigating their location in a network that “contains all possible substances” (2000, 72). Individual substances are the nodes, while the relations of production and mutual reaction form the connecting relations.

- Problem: not even remotely as fully worked out as microstructuralism

(2) Grounding substances in thermodynamics

- The thermodynamic behaviour of system depends on the number of distinct chemical substances present in it, which provides a criterion for when the substance is pure rather than mixed.

Position

"This, in turn, implies a criterion for sameness and difference for substances: Two bodies of stuff are the same chemical substance if they act as a substance when mixed; they are different chemical substances if they act as a mixture." (Hendry 2016, 270)

Let us consider three ways in which the **identity of substances could be grounded in thermodynamic properties**:

- 1 Some portion of matter is a mixture just in case it can be separated physically into different components (e.g. by heating, making the matter undergo phase transitions); if the composition is constant across phase transitions, the substance is pure.
 - both parts don't work (Ex: azeotropes)

(2) Grounding substances in thermodynamics

- 2 Use **Gibb's phase rule**, which related the number of components in a multiphase system to the number of phases present in it.
 - does not work (Ex: calcium carbonate)
- 3 Use **entropy of mixing**: samples are same substance if there is no entropy change on isothermal mixing, different if entropy increases.
 - problem: violates chemical practice (Ex: spin isomers)

Conclusion

The considered thermodynamic criteria of identifying substances "are not extensionally equivalent to those that chemistry has developed for itself, and which are reflected in its systems of naming and classification, and its theoretical explanations. The thermodynamic view of chemical sameness and difference is not the same as chemistry's." (Hendry 2016, 272)