# A Metaphysics for the Classification of Chemical Reactions in Practice

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I, Stephanie Ratcliffe, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

# *Abstract*

This thesis investigates the classification of chemical reactions in practice. It is motivated by the lack of discussion in the natural kind literature on the classification of reactions and other non-entity like things. I appeal to the discipline of chemoinformatics and study a new approach to the classification of reactions which is aimed specifically at meeting the needs of chemists in industry. I show that this methodology consists of three stages; the identification of a type of reaction of interest, the identification of a quantitative structural activity reaction and the importing of this data into a neural network. The output of classification is a reaction landscape which represents the similarity relations that hold between the different reactions.

My aim is to outline a metaphysics that is descriptively fit for purpose with respect to my case study. I argue that such a metaphysics must be descriptively accurate, capture appropriate similarity relations and promote explanatory unification. I evaluate the entities and activities ontology propose by Machamer, Darden and Craver, an ontology consisting on entities and dispositional properties and causal dispositionalism, against my criteria.

I argue that none of these accounts are descriptively fit for purpose and that commitment to an ontological category of processes is required alongside commitment to entities and dispositional properties. I suggest that the types of processes revealed in classification fall in the category of processes.

From my analysis of reaction classification throughout the course of my thesis, I generate a list of characteristics associated with reactions and use this to provide an account of the metaphysics underlying the category of processes. My proposal focuses on the relationship between potentiality and actuality in a given chemical reaction.

# Summary

This thesis investigates the most appropriate metaphysics for the classification of chemical reactions in chemical practice. In **chapter 1** I give an introduction to the notion of a chemical reaction and examine the ways in which chemical reactions are classified into types in everyday and scientific practice. I also introduce the different approaches to classification in the natural kind literature from social constructivism, weak realism to essentialism about natural kinds. My aim is to show that, as it stands, none of the current accounts of classification are able to accommodate the classification of reactions. This is firstly due to the accounts being primarily concerned with the classification of entities. Secondly, those accounts that do address the classification of reactions do not do so in a scientifically informed manner. For each account of classification I discuss the prospects for further development with respect to accommodating reaction classification in practice.

**Chapter 2** explores the classification of chemical reactions in practice and commits to a naturalized approach to metaphysics. I focus on the chemical discipline of chemoinformatics and the classification of organic and enzymatic reactions in order to meet demand from industry for better, more efficient reactions. I introduce a new methodology for classification which involves the search for quantitative structure activity relations in which lower level structural properties are associated with the instantiation of certain types of chemical reactions. I also describe the application of neural networking to provide a representation of a reaction landscape. This reaction landscape reveals the similarity relations that hold between reactions whilst clusters of reactions that correspond to a given type.

I conclude this discussion by highlighting three criteria that a metaphysics of the classification of reactions must meet if it is to be descriptively fit for purpose. These include; descriptive accuracy, capturing similarity relations and promoting explanatory unification and the fruitful development of science.

The discussion of chemical practice also allows me to conclude that social constructivism and strong essentialism are incompatible with classification in practice. This leaves several weak realist positions such as promiscuous realism, microstructuralism and homeostatic property cluster kinds that might be able to accommodate my case study. I identify that these positions commit to a range of different ontological components; entities, properties, processes and mechanisms. The remaining chapters will assess which components we must be ontologically committed to if we are to capture classification in practice. This discussion will help me outline my positive proposal in chapter 6.

In **chapter 3** I assess whether we can give a metaphysics of classification by appealing to mechanisms and, in particular, the entities activities ontology proposed by Machamer, Darden and Craver (MDC). I draw out the key features of activities and some of the advantages it has over an entities - dispositions ontology. I show that MDC use the term 'activities' in the same way as the chemists in my case study.

I argue that in order for the entities – activities ontology to meet the criteria of similarity it must be able to ground possibility statements concerning how reactions might proceed under a particular set of conditions. I undertake an interpretive project in which I suggest MDC intend a modal reading of activities and examine how to flesh out this claim. I argue that a modal reading of activities is not feasible because they lack the required amount of potentiality.

I suggest that MDC's account requires additional ontological commitment to dispositions in order to be fit for purpose. I show that making an explicit commitment to dispositional properties where these properties are attributed equal status to entities and activities best meets the criteria of descriptive accuracy and explanatory unification.

In **chapter 4** I examine whether the entities - dispositions ontology can accommodate the classification of reactions in practice. I begin by comparing the way in which chemists treat reactions in practice to the treatment of entities and dispositional properties in practice. I suggest that reactions are different to entities

in the sense that entities are wholly present whilst reactions have temporal intervals, reactions are also treated as the means by which entities change.

I suggest that reactions are like dispositions in the sense that they are potentials for something to happen. They are directed towards a certain end product and they bring about their own destruction as they cease to exist when the end product has occurred. However reactions are also unlike dispositions as they are associated with an actuality or active unfolding which can be measured and interfered with.

I also address whether reactions can be reduced to collections of entities and disposition. I show the restricted arity of dispositions means this isn't possible whilst preserving explanatory unification and adequately capturing similarity relations. I end by concluding that we must have access to processes amongst our ontological resources. One option is to commit to a third ontological category of processes. The second option in to investigate whether we can get access to processes at no extra ontological cost.

In **chapter 5** I investigate the possibility that the causal dispositionalist account can provide identity conditions for processes at no extra ontological cost in addition to dispositions thus meeting the demand for a more minimal ontology.

I introduce the disposes towards metaphor and the corresponding distinction between enabling conditions and causes. I show how, for the causal dispositionalist, enabling conditions place a limit on the transitivity and as a result are able to individuate causal processes. I go on to argue that the causal dispositionalist account is not descriptively fit for purpose. It fails to give a descriptively accurate account of how processes are identified in practice due to a discrepancy between the notion of *causing of an event* and the *causing of a process*. I also argue that the causal dispositionalist underplays the role of perspective when identifying processes in practice.

I add that the causal dispositionalist account also fails to capture similarity relations and promote explanatory unification. This is due to the dispose towards metaphor being vague and unconstrained meaning that any possible situation can be explained by the presence of a particular power. I argue that the attribution of powers should come with a specification of the conditions under which powers might be operative and the functions by which those powers combine. Mumford and Anjum appeal to functions that govern the combination of powers but tell us they should not be considered laws of nature. A more detailed account of the ontological status of functions is also crucial if the causal dispositionalist account is to be descriptively fit for purpose.

**In chapter 6** I outline my positive account for a metaphysics of classification of chemical reactions in practice. I propose a 3- category ontology consisting of entities, dispositional properties and processes where reactions fall into the category of processes.

I outline the metaphysics underlying my category of processes by appealing to an Aristotelian account of change that captures the relationship between potentiality and actuality in a given chemical reaction. On my account, a type of process is one where all token processes engage in the actualising of the specific potentiality that is associated with that process type. I show how my proposal captures the way in which reactions are both similar and different to dispositional properties.

I show two ways in which my account is different to the account of processes offered by Dupré. Firstly, unlike Dupré, I remain committed to entities. In addition, whilst my account of processes is similar in spirit to Dupré's, my account is able to account for the relation between potentiality and actuality associated with processes in the context of scientific examples. My account also has the advantage over Dupré's in that it can accommodate the types of reactions revealed in chemical classification, something which Dupré does not attempt. I end this chapter by offering a reason to believe my account has scope to be applicable beyond this particular aspect of scientific practice.

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*For Carolyn*

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# *Introduction*

Scientists have long sort to classify particulars into types. These efforts at categorisation have helped bring order to the world and direct scientific inquiry. Scientists have engaged in classification in the physical sciences through to the social sciences, with some philosophers asserting that in at least some of these cases the resulting types form natural kinds. For example, Russell (1905) took natural kinds to include '*dogs, wood, atoms, molecules, electrons, positrons, neurons and discrete energy levels,*' whilst Putnam (1975) famously refers to kinds of '*water, gold and tigers*'.

Just as philosophers disagree over whether beliefs, diseases, colours or species are natural kinds, they also disagree on how natural kinds should be defined. In virtue of what is a kind, a natural kind? Some philosophers have asserted that natural kinds possess a 'naturalness' that sets them apart from kinds that are mere artefacts. For example, Guttenplan (1994) asserts that 'to understand the concept of a natural kind, one must focus on the difference between kinds as represented by the set of typewriters and those as represented by the set of tigers' (Guttenplan, 1994, 449). There is a common set of properties that all typewriters have in virtue of being typewriters and this set of properties provides a degree of predictability about the way typewriters behave. Nonetheless typewriters do not occur in nature and so as Guttenplan points out they constitute artefacts rather than natural kinds. They lack the required 'naturalness'.

Traditionally the naturalness associated with natural kinds involves the notion that these kinds *cut nature at its joints*. Slater and Borgihini (2011) take Plato's metaphor to suggest that the world comes to us 'pre-divided' and our scientific theories are successful in so far as they reveal these divisions by carving nature at its joints. They add that that the categorisation of individuals into kinds represent

discoveries not inventions. In so far as scientific theories are successful, they latch on to an independent objective reality.

However LaPorte (2004) has argued that when considering the notion of 'naturalness' that is associated with natural kinds a more nuanced account is required;

> 'Not all human made kinds fail to be natural kinds. Humans have produced minerals such as quartz and diamond in the lab. Humans have also produced elements. Techenetoum is a synthetically produced element that has not been found to occur naturally on earth' (LaPorte, 2004, 18).

He also questions whether all things that exist in nature independently of humans should constitute natural kinds. He suggests that 'mud, slime or dust' are more like 'trash kinds' and should not be considered natural kinds. If natural kinds are not to be identified in virtue of their independent existence in nature then how should we proceed?

As indicated by Guttenplan, traditionally kinds are identified on the basis of members of that kind sharing a number of natural properties in common. These properties constitute sufficient and necessary conditions for kind membership and are referred to by some philosophers as essential properties. In virtue of these common properties, kinds are deemed to possess a high degree of projectability. In the case of gold, for example, we can make predictions about the density, melting point or conductivity of a token instance of gold in virtue of it having the 'essential property' atomic number 79.

Gold is a commonly cited example because this traditional conception of natural kinds is particularly applicable to chemistry, with the Periodic Table of Elements considered paradigmatic examples of natural kinds. Each element is identified according to its atomic number, where this constitutes sufficient and necessary conditions for membership of that natural kind of element. Interestingly, the history of the Periodic Table also reveals that classification is subject to revision. The Periodic Table was initially arranged according to atomic weight until it was established that a classification according to atomic number revealed more accurate

similarities and patterns of behaviours. Taking atomic number to constitute sufficient and necessary conditions for kind membership for elements involved an acceptance of isotopes. Isotopes possess additional neutrons and therefore have a higher atomic weight. Nonetheless, this lower level variation was permitted within natural kinds of element.

This traditional account of classification has been criticised for not accurately capturing classification in other areas of science. It is particularly problematic for biological kinds, where candidates for defining the extension of a kind include a shared ancestral history or a reproductive isolation. In addition, in the case of species, these two approaches are often in conflict with each other since it is possible for two organisms with no shared ancestral history to engage in interbreeding (Griffiths, 2011).

The philosophy of biology raises additional domain specific questions such as whether species constitute natural kinds at all. Similarly, the philosophy of psychology has addressed domain specific issues such as whether mental states constitute natural kinds. Questions concerning whether philosophical accounts of natural kinds are consistent with current scientific knowledge result from the increasing popularity of naturalized philosophy of science and metaphysics. This idea associated with Quine (1969) Sellars (1962) and more recently Ladyman and Ross (2007), suggests that the best evidence about the way the world is comes from science and so philosophers are wise to take this into account.

Related to the notion of naturalised philosophy of science and metaphysics is the turn to practice in the philosophy of science. The *Society for the Philosophy of Science in Practice* states in its Mission Statement;

> 'Philosophy of science has traditionally focused on the relation between scientific theories and the world, at the risk of disregarding scientific practice. We advocate a philosophy of scientific practice, based on an analytic framework that takes into consideration theory, practice and the world simultaneously' (Philosophy-science-practice.org, 2014).

Philosophy of science in practice has its origins in accounts of naturalised philosophy, but hadn't until recently entered the mainstream of philosophy of science. Lohkivi and Vikalemm (2012) describe this practical turn as the idea that we should be concerned not only with scientific theory but 'how science actually works'. Dupré, on the other hand identifies two ways of conducting philosophy of science in practice (Dupré, 2012). Firstly he identifies 'philosophy-of-science in practice' where this involves direct engagement and interaction between philosophers and scientists on philosophical problems or collaborations on a common question. These questions might concern 'background assumptions, logical structure, implications of unexpected or even undesired test results' (Boumans and Leonelli, 2013).

Alternatively, Dupré identifies philosophy of science-in-practice as the study of 'science in the making.' This addresses the everyday activities, aims, interests and methodology of science. Philosophy of science-in-practice does not necessarily require collaboration with scientists. My thesis certainly attempts to put into practice Dupré's second definition of philosophy of science in practice. I also take the issue of classification to be an important point of intersection between metaphysics and science and have attempted to produce a metaphysics of classification that meets the needs of scientific inquiry. Nonetheless, whilst my project has been influenced by scientists I do not claim that it is a collaboration.

My thesis examines the metaphysics of classification within chemistry. This is a particularly exciting project because the philosophy of chemistry remains a new and fruitful discipline. Chang (2012) Hendry (2008) (2010) and Needham (2000) (2004) (2011) have done important work in establishing the philosophy of chemistry in light of the anti-reductionist trend. This has involved addressing issues specific to chemistry such as the nature of substance, atomism and the chemical bond. They have also highlighted the lessons the philosophy of chemistry has for the philosophy of science more generally, with respect to issues such as realism, explanation and modelling.

I previously stated that chemistry has provided the paradigmatic example of classification via the Periodic Table of Elements. My aim is to push forward debate

regarding chemical classification by looking to current chemical practice. As I shall discuss in chapter 1, Hendry (2008) has already challenged the traditional conception of natural kinds by showing it to be problematic with respect to more complex chemical entities. My thesis will focus on another aspect of chemical practice which has been overlooked in discussions of classification; the chemical reaction.

I will begin in chapter 1 by giving a brief introduction to chemical reactions and identifying some familiar classifications of reactions. I then outline the key accounts of classification in the natural kind literature and show that most are directed towards the classification of entities. In addition, I show that those accounts that address the classification of processes do so in a scientifically uninformed manner. I assess the potential for each position to be adapted in order to accommodate the classification of reactions in practice.

In chapter 2 I begin the project of philosophy of science in practice. I describe how the classification of reactions has become an important aspect of chemical practice due to increased demand from industry for more efficient reactions with larger yields. In particular, I identify a demand for a better manipulability and control of chemical reactions. I describe a recently developed methodology for the classification of reactions and show how it is used to produce a more refined classification of enzymatic reactions. I use this discussion to draw out a number of constraints that a metaphysics compatible with chemical practice must meet. I call this kind of metaphysics *descriptively fit for purpose*. I argue that a metaphysics is descriptively fit for purpose with respect to my case study if it is descriptively accurate, captures appropriate similarity relations and promotes explanatory unification.

I suggest that the accounts of classification outlined in chapter 1 refer to a variety of ontological components such as entities, properties, processes or mechanisms. My strategy for adjudicating between these positions is to examine which ontological components are required to capture the classification of reactions. In chapter 3 I examine whether commitment to mechanisms by virtue of the entities - activities ontology is sufficient to capture the classification of chemical reactions in

a manner that is descriptively fit for purpose. In chapter 4 I examine the entities - dispositions ontology and in chapter 5 I assess causal dispositionalism against my criteria. In chapter 6 I give a positive proposal for a metaphysics for chemical reactions that is descriptively fit for purpose.

My ontological positive proposal is two-fold;

Part 1a: Realism about processes as a distinct ontological category is necessary

Part 1b: Realism about the ontological category of entities and the ontological category of dispositional properties is also necessary in addition to the category of processes. None of these categories are on their own sufficient to capture classification of reactions in practice

Part 2: A type of process is one where all token processes engage in the actualising of the potentiality that is associated with that type

# Chapter 1: Accounts of Classification and Classifying Reactions

## 1:1: Introduction

A central aspect of scientific activity is the classification of token instances of a phenomenon into types on the basis of the similarities that members of that type bear to one another. In the philosophy of science and the metaphysics of science such groupings or types can be referred to as natural kinds. There are many approaches to a philosophical account of classification and different philosophers have different things in mind when they refer to a 'natural kind'. The details of each account will depend on the proponent's particular philosophical and metaphysical position. The purpose of this chapter is to provide an overview of the different positions concerning classification systems in the philosophy and metaphysics of science. The process of examining the nuances of existing positions is crucial to understanding which account, if any, is able to accommodate the classification of reactions in practice.

When thinking about the different positions one could take with respect to natural kinds it is helpful to draw a distinction between natural groupings or classifications and 'natural kinds' construed as entities. Constructivists about kinds are anti-realist with respect to both options; they deny that there exists an objectively natural means of classification and they take the kinds identified by empirical inquiry to be interest dependent (Kukla, 2001). At the other end of the spectrum are strong essentialists who commit to the existence of natural kind entities which themselves have an essence. These essences consist of necessary and sufficient conditions for kind membership that correspond to the natural groupings identified by science (Ellis, 2001). Between constructivism and essentialism lie a variety of realist positions about natural kind classification which commit, to different

degrees and by different means, to the existence of objectively natural groupings (Boyd, 1991 & Dupré 2003).

In addition to outlining these positions this chapter will raise the concern that the natural kind literature is preoccupied with the classification of entities and objects; the paradigmatic examples of classification being gold, water and tigers.[1] I take this to be problematic on the grounds that chemists also classify instances of other chemical phenomena into groups on the basis of the similarities they have to each other, however these other phenomena are not typically construed as entities. My thesis focuses on the classification of reactions although there may be other scientific phenomena that do not fall into the entities and objects paradigm but still undergo classification as a part of scientific practice. Other examples might include chemical phenomena where a change occurs but the atoms and bonds do not undergo rearrangement such as dissolution, heating, evaporation. I shall not discuss these cases in any detail.

I suggest that we should aim to provide an adequate philosophical account of classification for all instances in which it occurs in science.[2] Even if we were to accept a disunified picture such that an account of the classification of reactions is different from an account of the classification of entities the onus is on philosophers to fill this theoretical hole.

I will begin this chapter with a brief introduction to the notion of a chemical reaction and will examine some of the ways in which reactions are commonly categorised into types. This discussion provides initial examples with which to examine the philosophical accounts of classification which I will outline in sections 1.3 – 1.9. I begin in section 1.3 with social constructivism. In section 1.4 I examine semantic essentialism followed by metaphysical essentialism in section 1.5. In section 1.6 I discuss Quine's weak realism about classification, in section 1.7 I address Boyd's homeostatic property cluster kinds and in section 1.8 I examine Dupré's

[1] This is with the exception of Brian Ellis' Scientific Essentialism which I shall discuss in section 1.5

promiscuous realism. Finally, in section 1.9 I focus in on debates about classification within the philosophy of chemistry.

## 1:2: Chemical Reaction

A chemical reaction is described in the IUPAC Compendium of chemical terminology as follows;

> ‘a process that results in the inter conversion of chemical species. Chemical reactions may be elementary reactions or stepwise reactions. Detectable chemical reactions normally involve sets of molecular entities as indicated by this definition, but it is often conceptually convenient to use the term also for changes involving single molecular entities (i.e. 'microscopic chemical events')’ *IUPAC, Compendium of Chemical Terminology, 2nd ed. (the "Gold Book") (1997). Online corrected version: (2006–) "chemical reaction".*

A reaction is described in terms of a reaction equation. Chemical reaction equations consist of a chemical formula or structural representation of the reactants on the left hand side and a chemical formula or structural representation of products on the right. They are separated by an arrow which describes the direction of the reaction. Equations should be balanced according to the stoichiometry i.e. the number of atoms of each substance should be the same on each side of the equation. Reaction equations for more complex reactions also indicate the transition states between reactants and products.

Chemists sometimes refer to the reaction centre and this includes all the parts of the entities that have bonds broken and formed during the course of the reaction. Typically, chemical reactions involve changes in the positions of electrons as a result of the breaking and making of chemical bonds between atoms; these are known as electronic changes. Nuclear changes, i.e. changes to the nucleus of reactions are only relevant to the sub discipline of nuclear chemistry which deals with chemical reactions between unstable elements.

As the definition above indicates reactions are typically characterised in terms of their reaction mechanism; this gives a step by step account of how the atoms and

bonds involved in the reaction rearrange themselves. However, to focus solely on the reaction mechanism is to only tell half the story. In any one reaction, many instances of the reaction mechanism will occur with the exact number depending on the amount of reactants used. In a reaction in which one mole of two reactants are used then there will be a total of 2 x 6.02214129(27) $\times 10^{23}$ entities involved in the reaction.

The domains of chemical kinetics and chemical thermodynamics describe the properties of the reaction as a whole focusing on the many reaction mechanisms taken together, rather than the individual reaction mechanisms. This is important for explaining and predicting features such as the rate of reaction, the activation energy required for the reaction to begin and the conditions for optimum yield. The rate at which reactants are turned into products is studied by chemical kinetics. Variables such as increased reactant concentration, increased surface area, increased temperature and pressure are known to increase the rate of reaction.

As I previously discussed, the periodic table of elements has provided the paradigmatic account of natural kind classification however contemporary chemistry is no longer primarily concerned with the identification and classification of static entities such as these. It is stated that; 'Chemistry deals with compounds and their properties and their transformations, thus, two objects have to be considered, compounds and chemical reactions, the static and dynamic aspects of chemistry' (Gasteiger and Engel, 2008, 1). In addition, with the ever expanding numbers of chemical reactions being discovered, the question of how to classify has become an important issue in organic chemistry. Writing in the Journal of Chemical Information and Computer Science in 1984, Hermann-Winter noted that;

> 'organic chemistry has grown to the point where there is an overwhelming number of known reactions and syntheses, hence the problem of classifying these reactions has become much more important. To classify means to develop general categories and gather related single items under these classes. Such generalizations specify a mechanistic explanation in terms of intermediates such as ions and radicals.' (Herman-Winter, 1984, 263).

More recently it was stated that;

> 'Classification of enzymatic reactions is required for genome-scale reconstruction (or comparison) of metabolic pathways, computer-aided validation of classification systems, or comparison of enzymatic mechanisms' (Diogo A. R. S. Latino, João Aires-de-Sousa, 2010, 325).

The classification of chemical reaction is common to scientific practice as well as our everyday interactions with reactions. Six of the most basic types of reactions have been identified as follows:

- Decomposition reactions involve a complex substance breaking down into more simple parts

  AB → A + B
- Synthesis reactions occur when two or more compounds combine to form a more complex substance

  A + B → AB
- Single displacement reactions occur when one element trades places with another element in a compound.

  A + BC → AC + B
- Double displacement reactions occur when two different elements switch places, forming two different compounds.

  AB + CD → AD + CB

More complex types of reactions include the following:

- Precipitation reactions are aqueous reactions that involve the formation of a precipitate or insoluble substance in the liquid.

  soluble molecule + soluble molecule -> insoluble molecule
- Neutralization Reactions are a special type of double displacement reaction that involves the reaction between an acid and base to form a salt and water.

  acid + base → salt + water
- Combustion Reactions occur when a hydrocarbon combines with oxygen to produce carbon dioxide and water.

  hydrocarbon + oxygen → carbon dioxide + water

- Hydrolysis reactions involve the breaking of chemical bonds by the addition of water.
- Polymerization is a type of chemical reaction that occurs when monomer molecules combine together to form polymer chains or three-dimensional networks.

  There are many forms of polymerization and different systems exist to categorize them.
- Photosynthesis reactions occur in all plant life. Carbon dioxide and water react with energy from the sun to produce glucose, oxygen and water

  $6\ CO_2 + 12\ H_2O + \text{photons} \rightarrow C_6H_{12}O_6 + 6O_2 + 6H_2$

The types of reactions outlined above can be instanced by different token entities and in some cases different types of entities at different times. In addition, it is possible that certain token instances will fall into more than one category, for example, each photosynthesis reaction is also a double displacement reaction. I have already hinted that the classification of reactions into kinds is an integral part of chemical practice and these are just some of the types of chemical reactions that we are most familiar with. I will begin to examine whether the types of reactions discussed above can be accommodated by the literature on natural kind classification.

## 1:3: Social Constructivism

Firstly consider the social constructivist's approach to classification. The constructivist denies that the classification of scientific phenomena into natural kind groupings is 'natural,' or latches on to the causal structure of the world. This is because, according to the constructivist, the classification process is too heavily dependent on human action and influence; Kukla states: 'X is said to be constructed if it's produced by intentional activity' (Kukla, 2000, 3).

Scientific constructivism can be divided into strong and weaker varieties. Weak constructivism does not deny that there exists an objective classificatory

system but maintains that it is out of our epistemic reach. This is the view associated with Locke when he makes his distinction between real and nominal essence. He argues that we classify entities according to their observable properties and as a result decisions about how to carve things up are based on convention i.e. the application of human concepts, interests and activities. Nonetheless, Locke also commits to the idea that kinds have real essences that depend on their microstructure. A system of classification based on real essences would, according to Locke, be objectively real if access to it were not beyond the scope of science.

A stronger form of constructivism is of the metaphysical variety which Hacking describes as follows;

> 'Constructivists tend to maintain that classifications are not determined by how the world is, but are convenient ways in which to represent it. They maintain that the world does not come quietly wrapped up in facts. Facts are the consequences of ways in which we represent the world' (Hacking, 1999, 33).

Strong constructivists deny there is an objectively real system of classification and as a result there is no reason to believe classification based on scientific inquiry is any more real than that which is made on religious or political grounds. There are at least two ways in which human interests affect classification according to the constructivist; causal constructivism and social constructivism.

## 1:3:1: Causal Constructivism

In the case of causal constructivism, X causally constructs Y if and only if X causes Y to exist, or to persist, or X controls the kind-typical properties of Y. The idea is that natural kinds are causally dependent upon human interests so that in advancing our own classificatory system we cause some change in the objects we are interested in via a feedback loop. For instance, in classifying x as kind K we cause some change in x such that as a result it comes to possess some additional properties which then in turn have a bearing on the extension of K. An example of this is the kind 'multiple personality disorder' which is described by Hacking and further

explored by Ali Khalidi (Ali Khalidi, 2010, 241). When an individual is classified as falling within the extension of this kind, they come to identify with the kind 'multiple personality disorder' and as a result tend to develop additional properties that further distinguish them from individuals that do not fall in this extension. These new properties are then fed back into the definition of the kind which is used for classifying further cases of multiple personality disorder and therefore the loop continues.

### 1:3:2: Constitutive Constructivism

The second way human interests influence classificatory practice is known as constitutive construction. X constitutively constructs Y if and only if X's conceptual or social activity regarding Y is necessary for Y to be a Y. The constitutive dependence of science on human interests maintains that 'what we call "facts about the world" are revealed to be facts about human activity' (Kukla, 2000, 21). For instance it might be argued that the notion of gender is constructed in this way since we can imagine a society that evolved in such a way that there existed no gender distinction over and above the distinction based on sex.

Since constructivists reject realism about the classification of entities they would, for the same reasons, deny realism about the classification of reactions. There is nothing about the position itself that indicates that a constructivist about classifications of entities should be realist about classifications of reactions. The question of whether constructivism is applicable to the classification of chemical reactions in practice will require a detailed examination of the methodology and the aims and interests behind each classificatory investigation. I will return to these considerations in chapter 2.

## 1:4: Semantic Essentialism

Essentialism about natural kind classification lies at the opposite end of the spectrum to constructivism. It is the thesis that for any kind, there are certain

properties that must be possessed by individuals in order for those individuals to qualify as members of that kind; these are known as essential properties. Some essentialists make the stronger claim that natural kinds themselves have essences. In this section I will discuss attempts to arrive at essentialist conclusions from commitment to semantic externalism in the philosophy of language.

The rise of essentialism is associated with the independent development of semantic accounts of reference by Putnam (1973) (1975) and Kripke (1972). Both were responding to Frege (1892) and Russell's (1905) descriptivist accounts of meaning in which names were taken to be abbreviations for definite descriptions which provide the sense of the name and determine what it refers to . A consequence of Frege's account is that meanings are 'in the head' in the sense that grasping a meaning is a psychological event. Putnam and Kripke's versions of semantic externalism challenged this intuition and, as I shall discuss in the following sections, are thought to lend support to essentialism.

## 1:4:1: Putnam's Account of Meaning

Putnam's Twin Earth thought experiment is his key motivation for semantic externalism. He asks us to imagine another possible world in which there is a planet named Twin Earth which is identical to Earth in all but a few respects. One of the differences is that the substance that is called 'water' on Twin Earth does not consist of $H_2O$ but XYZ, nonetheless $H_2O$ and XYZ share identical macro properties, they both boil at 100˚C and are found in lakes and rivers etc.

Putnam then asks us to imagine a time before the development of modern chemistry in which the microstructure of water on each planet was unknown. Oscar is an Earthian in 1750 and $Oscar_1$ is his twin Earthian duplicate. They are both identical in terms of psychology. When confronted with the white colourless liquid known as 'water' in their respective worlds they will be in the same psychological state with regards to it, yet 'water' has different extensions in each case, $H_2O$ for Oscar and XYZ for $Oscar_1$. It is just that each is unaware of the exact extension of the

term in question. As a result Putnam concludes that psychological states cannot determine extension (Putnam, 1975, 140).

His argument rests on the notion that kind terms such as water have an indexical quality and so when we want to express what we mean by terms like 'water', we give an ostensive definition, i.e. we say 'this liquid here is water'. There are two potential implications of this for a theory of meaning. Consider a situation in which there are two worlds in which I and my double exist; $W_1$ is the actual world and $W_2$ is another possible world. In both worlds I point at the glass and say 'this is water;' in $W_1$ the glass contains $H_2O$ and in $W_2$ the glass contains XYZ. We could maintain that water means the same thing in both worlds but it's just that water is $H_2O$ in $W_1$ and water is XYZ in $W_2$. In this case 'water' would be world relative and constant in meaning. Putnam argues that this account is mistaken and instead we should consider water to be $H_2O$ in all possible worlds and concede that "water" doesn't have the same meaning in all possible worlds.

He defends this conclusion by asserting that when I say 'this is water' the explanatory power lies in the fact that 'water' is considered to be whatever bears a certain sameness relation to what we call water in the actual world. It doesn't matter if we are unable to specify the nature of this relation; identifying the sameness relation is an epistemic problem and it is revisable in the light of new evidence (Putnam, 1975, 140).

Putnam adds that not all ordinary speakers need to be aware of the sameness relation in order to correctly use the term; he points to a linguistic division of labour such that we recourse to an appropriate expert where necessary. Putnam's account still allows for a description to be associated with a term; this forms part of his meaning vector and includes all the stereotypical features associated with the term by the linguistic community although it plays no role in determining the extension of the term.

It is the idea that the 'same L' relation is a cross world equivalence relation that motivates essentialism. Were this to be the case then it would follow that there

is no possible world in which something either has the appropriate property (L) and fails to be a member of that kind or is a member of the kind without possessing it. As a result it is assumed that 'same L' is the essential feature of the kind in question.

The possibility of deriving essentialist conclusions by appealing to Putnam's cross world sameness equivalence relation has been criticized by Mellor who argues that the approach is question begging (Mellor, 1977, 300). He argues that even if we accept that reference is fixed on the basis of a sameness relation that holds between individuals of the same kind across possible worlds, it does not follow that these individuals must share the same all the properties in common. He asks us to conceive of a case in which water has 10 'important' properties but could lack any one of them and still be water; in this case only the disjunction of all conjunctions of nine of them is essential to water. But then the sameness relation would not be one of equivalence since it is not transitive; it would be possible for a sample of water in another possible world to lack any one of the properties of water in the actual world. Mellor adds that the only way in which essentialism might follow from the notion of a sameness relation would require prior acceptance of essentialist conclusions; i.e. the requirement that possession of a common property is a requirement of kind membership (Mellor, 1977, 307).

Mellor also objects to the anti-descriptivist conclusions Putnam draws from the Twin Earth thought experiment on the grounds that they too rest on a hidden essentialist premise. He rejects the conclusion of the Twin Earth thought experiment that meanings are not in the head because he rejects the premise that water on Earth and Twin Earth have different extension. This premise, according to Mellor begs the question. Why must they have different extensions, he asks; 'Because its microstructure is an essential property of water? Well, that is what's in question' (Mellor, 1977, 303). If extension is determined by beliefs and Earthians and Twin Earthians have the same beliefs about the substance then the fact that they have different microstructures is of no concern. He argues contrary to Putnam, that 'water' has the same extension on Twin Earth and Earth in both 1700 and 1900

(Mellor, 1977, 303). Earthians and Twin Earthians always have and continue to mean the same thing by the term 'water.'

> 'It is indeed quite plain to my Fregean eye that in 1950, as in 1750, 'water' had the same extension on Twin Earth as it had here. There was water on both planets alike, and there still is. We simply discovered that not all water has the same microstructure' (Mellor, 1977, 303).

To put it another way he believes that we have discovered that local varieties of water vary in microstructure, but that this has no impact on the extension of the term unless a form of microstructural essentialism is presupposed. Thus Mellor concludes that Putnam has not shown that it is possible to be in the same psychological states with respect to two substances that have different extensions and therefore he is not justified in his rejection of a Fregean account of meaning (Mellor, 1977, 309). Therefore he also rejects the claim the Putnam has provided independent justification for essentialism.

### 1:4:2: Kripke's Account of Meaning

Kripke's version of semantic externalism is also motivated by what he takes to be inadequacies with the descriptivist theory of meaning and specifically with its metaphysical consequences (Kripke, 1981, 113). Consider the case in which 'John' designates an individual and 'α' is the set of properties associated with John. On the descriptivist picture it is the case that sense determines extension and so it follows that, 'necessarily if John exists, John has most of the properties 'α''. Kripke argues that this is false since even if John does possess most of the properties 'α', he might not have done. The difficulty lies in the fact that, names behave differently from descriptions in modal contexts. For example, 'necessarily Elizabeth II is the Queen of England,' is false since we can imagine a possible world in which she abdicated from her position, but the statement 'necessarily the Queen of England is the queen of England' is true (Kripke, 1981, 113). The reason for this is that names are rigid designators; they refer to the same entity in all possible worlds in which that entity exists and they never refer to anything else. Most definite descriptions, on the other

hand, are not rigid designators. Consequently, Kripke argues that names and definite descriptions cannot ordinarily be equated (Kripke, 1981, 48). Kripke extends the notion of a rigid designator to apply not just to proper names but also to selected definite descriptions; those descriptions that scientists associate with natural kind terms. In both cases the concept of rigid designation has important philosophical consequences.

In the case of proper names, Kripke's case of Hesperus and Phosphorus provides an example of a necessary a posteriori statement since both 'Hesperus' and 'Phosphorus' both rigidly designate Venus and this was discovered to be the case. The same idea applies to theoretical identity statements involving certain definite descriptions such as 'gold = atomic number 79'. If 'gold' and 'atomic number 79' are both rigid designators then if it is true that 'gold = atomic number 79' in one possible world, then it must be the case across all possible worlds, i.e. the statement is necessarily true if true at all.

This motivates essentialism since that if it is necessary that anything we call 'gold' has atomic number 79, then this serves as an essential condition for membership of the kind gold. Even if by itself it does not constitute a sufficient condition on kind membership, we can assert that it is essential to gold that it has atomic number 79.

Whilst rigid designation provides an intuitively appealing argument for essentialism, attempts to derive essentialism from rigid designation have been shown to be problematic. As with Putnam's account the key objection is that such attempts rely on a trivial essentialist premise. This problem is described by Mellor who asks us to imagine that 'water' and '$H_2O$' are rigid designators and then asks what is required in order to construct the identity statement 'water is $H_2O$' (Mellor, 1977, 307). His answer is that 'water' and '$H_2O$' must be coextensive in all possible worlds. Formulated in this way the identity statement trivially entails essentialism since it requires that all samples of water, in all possible worlds are also samples of $H_2O$. Therefore, by definition $H_2O$ would be essential to water. Nothing about the necessity of the identity statement 'water is $H_2O$' entails that being $H_2O$ is an

essential property of water; rather this is a requirement on the formulation of the identity statement in the first place (Mellor, 1977, 307).

In addition, Kripke's footnote 56 attempts to derive a special instance of essentialism from rigid designation. This has been discussed by Salmon who shows the proof to be problematic and concludes that essentialism cannot be derived from semantic considerations (Salmon, 1979, 703- 725). The particular essentialist conclusion that Kripke hoped to derive in this case is that *if a wooden table has its origins from a certain hunk of wood then it could not have had its origin in any other hunk of wood.* If successful then the strategy could be extended to give stronger essentialist conclusions about natural kinds (Kripke, 1981, 114). The proof goes as follows:

*Let B name a table and A name a hunk of matter from which table B is constructed in World 1 (W1) and let C be the name of some distinct hunk of matter that also exists in W1.*

Kripke wants to show C1: ~◊ (B,C) that it is impossible for table B to originate from hunk C. It follows from this that if it is possible for a given table to originate from a certain hunk of matter, then it is necessary that the table originate from that very hunk of matter. Salmon formulates Kripke's first premise as;

P1: For any table B and any hunks of matter A and C, if it is possible for any table B to be originally constructed entirely from hunk A while hunk C' does not overlap with hunk A, then it is also possible for table B to be originally constructed entirely from hunk A while some other table D distinct from B is simultaneously originally constructed entirely from hunk A' (Salmon, 1979, 708).

The proof also requires the necessity of distinctness which states that, if things are not identical then they could not have been identical and as a result it is possible to construct two tables, simultaneously from distinct hunks of wood (Salmon, 1979, 709). Using P1 and the necessity of distinctness, however, Kripke does not derive his desired C1 but C2;

C2: $\Box[T(D,C) \rightarrow D \neq B]$;

C2 states that necessarily even if a new table, D, was made from hunk of matter C and no table were made from A, D would not be B. Even if hunk of matter A did not exist, it still would not be the case that D would be identical to B. To complete his proof it must be possible to derive;

C1: $\sim\Diamond(B,C)$

or

C3 $\Box(x)[T(x, C) \rightarrow x \neq B]$

since C3, the claim that in any possible world in which a table is constructed from hunks C, the table constructed from hunk C is still not table B, is trivially equivalent to C1. Salmon maintains that in order to reach the required conclusion Kripke is forced to make use of a hidden premise, P2;

P2 If it is possible for a table x to originate from a hunk of matter y then necessarily, any table originating from hunk y is the very same table x and no other (Salmon, 1979, 711).

P1, P2 and the necessity of distinctness yield the conclusion that if it is possible for a given table to originate from a certain hunk of matter then it is necessary that the given table does not originate from any non-overlapping hunk of matter. For instance;

1. Let W1 be a possible world in which an arbitrary table B originates from some hunk of matter A

2. Let C be any hunk of matter that does not overlap with A in W1

3. By P1 there is a possible world in which table B originates from A and a second table called D originates from C.

4. By the necessity of identity and distinctness tables B and D are distinct in every possible world, *(if is the case that they are distinct in W2 they must be distinct in the actual world otherwise they would be identical in every possible world*)

5. In an arbitrary possible world in which some table is constructed form hunk C, given P2, this could not be table B from W1. *(This is because, according to P2 the table in question in W3 is table D, and B and D are distinct in every possible world including world 3).*

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6. Therefore there is no possible world in which table B originates from hunk C.

P2 is crucial to the argument however using P2 begs the question since it is an essentialist principle. It asserts that if a given table x is such that it might have originated from a certain hunk of matter y then the table has as an essential property, the feature that no other table distinct from it originates from y. According to Salmon, Kripke's derivation of essentialism from the causal theory of reference works only in virtue of containing essentialism amongst its premises. Consequently Kripke's derivation does not go through. (Salmon, 1979, 712).

Thus far it's been established that essentialism cannot be non-trivially derived from rigid designation, however Kripke employs a second strategy that motivates essentialism by appealing to our modal intuitions. He asks us to consider a situation in which it is revealed that the stuff we have, up until now, referred to as gold is in fact blue and only appears gold as a result of an optical illusion. Kripke suggests our intuitive response would be to assert that the stuff we call gold is still gold and to state in addition, that gold is not always yellow (Kripke, 1972, 118). He supports this claim by referring to the distinction between those properties that fix reference for a given linguistic community and those properties that constitute the essential nature of the kind.

Kripke then extends the scope of the intuition by appealing to a counterfactual situation in which fool's gold is found in another possible world in the

exact same location as true gold is found in the actual world. Consequently, the only difference between the two substances is that one lacks the property of having atomic number 79 (Kripke, 1972, 119). Nonetheless, Kripke maintains that this new substance is still not gold on the grounds that it lacks the appropriate microstructure. Kripke concludes that it is necessary and not contingent that gold be an element with atomic number 79 such that the possession of this property is an essential property of gold.

One of the reasons that these modal intuitions are appealing for the essentialist has to do with explanatory priority. In the case of gold, gold's atomic number functions in explanations of its density and reactivity while the reverse does not hold, thus it is intuitive to consider atomic number to be more significant than other properties.

Mellor has argued that this strategy for motivating essentialism is flawed (Mellor, 1977, 307). Consider Quine's criterion for ontological commitment; 'A first-order sentence carries commitment to Fs just in case Fs must be counted amongst the values of the variables in order for the sentence to be true' (Quine, 1948, 32). Quine requires that we should only be committed to things that we must refer to in order to state what is true. However, if this is combined with the micro reductive trend that advocates the explanation of things in terms of their smallest possible parts then it seems that we can replace reference to the thing in question with reference to their parts. In other words we can replace a reference to water with a reference to $H_2O$ and so it follows that being $H_2O$ is essential to water.

However if we are to replace reference to water with reference to $H_2O$ then it must be the case that all properties of water are deducible from $H_2O$ with the consequence that in any possible world in which $H_2O$ is present the other properties associated with water must also be present. But were this to be the case then all the properties of water would be deemed essential to it and the essentialist cause isn't furthered. Alternatively if macro properties of water cannot be deduced from $H_2O$ then reference to them cannot be replaced with $H_2O$ and so the essentialist argument

fails again.[3] Thus attempts to motivate essentialism on the basis of considerations stemming from rigid designation or scientific explanation are spurious.

## 1:4:3: Semantic Essentialism and Classifying Reactions

My aim in this section has been to outline the dialectic between semantic essentialists and their opponents. This is to allow for an analysis in chapter 2 of whether essentialist intuitions are shared by chemists investigating the classification of reactions in practice. Initially it seems that to the extent that the arguments above provide motivation for essentialism about entities they might also indicate essentialism about reactions.

I suggest that the essentialist intuitions of Putnam and Kripke can be applied to chemical reactions. Consider Putnam's Twin Earth thought experiment. Rather than asking us to consider an entity with a certain microstructure on Twin Earth we might instead consider a combustion reaction such as the burning of methane to give carbon dioxide and water. On earth the reaction has the following chemical equation:

$CH_4 + 2O_2 \rightarrow CO_2 + H_2O$

The reaction occurs because heat energy is input into the system. The carbon atom is oxidised and loses electrons to form carbon dioxide and the oxygen is reduced i.e. it gains electrons to form water.

We can recreate a semantic essentialist argument about reactions by appealing to a thought experiment inspired by Handfield (Handfield, 2010, 1). We can imagine a situation in which the reaction appeals to take place on Twin Earth except the atoms involved in the reaction on Twin Earth have an invisible protective layer with absorbs the heat and protects this input energy from breaking down their bonds. Instead the bond between the atoms are broken down by 'nano-machines' which separate the atoms and rearrange them to produce carbon dioxide and water.

[3] This objection applies to those who reach essentialist conclusions on either the Kripke or Putnam's account of reference.

In this case it seems that the start and termination conditions of the reaction are the same but the way in which the termination conditions were achieved were very different to the combustion of methane on earth. It's not clear that this is an instance of combustion and this may add weight to the notion that reactions have an essential structure.[4]

The thought experiment raises a number of questions for the classification of reactions; firstly is it the case that reactions are classified on the basis of the structure of reaction; if so how do chemists use structure to specify necessary and sufficient conditions for kind membership? What is a sufficient degree of structural similarity for two reactions to be of the same kind? In chapter 2 I will attempt to answer these questions and assess whether this essentialist intuition applies to the classification of more complex reactions.

## 1:5: Metaphysical Essentialism

In the previous section I examined the variety of essentialism that results from semantic considerations and whether such arguments are viable. In this section I will address metaphysical essentialism which differs from semantic essentialism in that it takes it as an assumption that the essentialist position is correct. In particular I will focus on Brian Ellis' metaphysical framework known as scientific essentialism (Ellis 2001, 2002). His thesis is that natural kinds are the prior and fundamental element of ontology, he also takes the essential properties of natural kinds to necessitate laws of nature with the implication that for Ellis laws of nature are metaphysically necessary (Ellis 2001, 2002).

### 1:5:1: Motivation

Ellis's scientific essentialism is developed in response to the metaphysical frameworks of Lewis and Armstrong. As I will discuss in this section Lewis and

[4] This thought experiment has been adapted from Handfield 2010 that applied to the case of dissolution of salt in water

Armstrong argue in different ways that laws of nature are contingent and natural kinds are supervenient on natural properties and so do not require a distinct ontological category.

Central to Lewis's account of laws of nature is his commitment to modal realism i.e. realism about possible worlds construed as concrete entities such that the notion of the actual world is indexical and relative to the speaker. This allows him to draw a distinction between metaphysical necessity which is achieved by quantifying over all possible worlds and nomological necessity which quantifies over worlds with laws of nature like the actual world. Thus P is metaphysically necessary if P is true in all possible worlds while P is nomologically necessary if it is true in all possible worlds that are nomically accessible from the actual world.

Lewis's anti-realism about necessity and laws of nature follows from his Humean supervenience which states that

> 'all there is to the world is a vast mosaic of local matters of particular fact, just one little thing and then another. [. . . ]For short: we have an arrangement of qualities. And that is all. There is no difference without difference in the arrangement of qualities. All else supervenes on that' (Lewis, 1986b, ix f).

Lewis reads this as the claim that all we need to be ontologically committed to is qualities and all else supervenes on them and there are no necessary connections between the various qualities. Consequently, he asserts that laws of nature are the regularities that hold between the qualities in the actual world, there are other possible worlds in which such regularities do not hold and so laws of nature are contingent. Lewis illustrates with the law like generalization that *if I eat bread then I will avoid starving* and asserts that there are worlds in which this regularity fails to hold such that I continue to eat bread but still starve (Lewis, 1986a, 91). This idea is captured in Lewis's principle of recombination; 'Roughly speaking, the principle is that anything can coexist with anything else, at least provided they occupy distinct spatiotemporal positions. Likewise, anything can fail to coexist with anything else' (Lewis, 1986a, 91).

With this in mind Lewis proposes the best systems approach to laws of nature on which he identifies collections or systems of truths and argues that laws of nature are provided by the system that best combines simplicity and strength. Strong truths are those that tell us a lot about the world. What it is to be a simple truth, however, is fleshed out by drawing a distinction between sparse and abundant properties. He takes the simplicity of a claim to be indicated by how easily it can be stated in a language where all predicates denote *sparse* properties as discussed below.

Lewis takes a property to be the set of all of its instances over all possible worlds and a relation to consist of an ordered pair of related things where its relation is considered to be the set of all of its instances across all possible worlds (Lewis, 1986a, 91). With this in mind he distinguishes between sparse and abundant properties. Abundant properties are those that provide the semantic value to the terms we use in everyday language, they are disjunctive, gerrymandered and give no indication of the qualitative similarity of those things who have the particular property in common. A small minority of all properties qualify as sparse properties, they are intrinsic, specific rather than gerrymandered and on Lewis's view they cut nature at its joints, such that the sharing of sparse properties is responsible for the qualitative similarities that exist between individuals. This last claim is fleshed out by construing properties as universals such that sharing a common property requires instantiating the same universal. While all natural properties are intrinsic on Lewis account it is not the case that all intrinsic properties are natural since a disjunctive property may be intrinsic if its disjuncts are also intrinsic.

For Lewis naturalness comes in degrees. He takes sparse properties to be perfectly natural properties and states that these are those properties that are revealed to us by fundamental physics. All other properties fall along the naturalness continuum depending on how directly they can be related to fundamental properties along chains of definability. Lewis states; 'Among all the countless things and classes that there are, most are miscellaneous, gerrymandered, ill demarcated. Only an elite minority are carved at the joints' (Lewis, 2984, 227).

Thus it is sparse properties that carve nature at its joints. The account of properties just outlined allows Lewis to flesh out what it is to be a simple truth as is required by his account of laws of nature. His account of fundamental properties also provides the basis on which he rejects ontological commitment to kinds.

Lewis suggests a reductive analysis of kinds in terms of natural properties such that two objects are members of the same kind if they possess the same perfectly natural properties. Kinds which are formed from conjunctions of properties derive their naturalness from the naturalness of their constitutive properties. As a result Lewis argues that any commitment to kinds over and above natural properties is redundant; the perfectly natural kinds are just the perfectly natural properties (Lewis, 1986b). Importantly, Lewis takes properties to be causally inert where regularities that hold between give rise to dispositional properties. Thus supervenient kinds do not have dispositional properties essentially.

Ellis' Scientific Essentialism also rejects the contingency of laws and supervenience of kinds that is postulated by Armstrong. In *A World of States of Affairs (1997)* Armstrong argues that the world is the totality of all states of affairs where a state of affairs exists if and only if a property holds of a particular, or a relation holds between two particulars, where properties and relations are taken to be universals (Armstrong, 1997, 20). Armstrong adds that states of affairs are ontologically prior to their constituents since neither properties, relations, nor particulars can exist independently of states of affairs.

For Armstrong nomological possibilities arise from combinations of universals and bare particulars into states of affairs. Consequently he identifies laws of nature with second order universals that hold between universals, that is, Fs are Gs is a law iff N(F, G) (Armstrong, 1983, 85). Nonetheless this relation is a contingent one; if it is a law that the heating of a metal is followed by the metal expanding it is possible that the N universal that relates them fails to hold and so the law might not hold.

Armstrong differs from Lewis in the sense that he has a more liberal conception of natural properties. He is committed to complex properties and

relations, arguing against the claim that all universals are simple. Complex property universals are formed from conjunctions of simpler properties. For example, given that F and G are distinct universals then (F&G) qualifies as a universal provided there is always some particular that instantiates both F and G (Armstrong, 1997, 31). Armstrong rejects the claim that complex properties supervene on their conjuncts and amount to no addition of being on the basis of the distinction he draws between basic co-instantiation and synergistic co-instantiation. In the latter case the power of the conjunction is either more or less than the sum of the power of the conjuncts. Complex properties involve the second type of instantiation, on this basis we must commit to conjunctive universals; they have non reductive causal powers (Armstrong, 1997, 34).

Similarly to Lewis, Armstrong rejects any commitment to natural kinds as universals. He argues that kinds supervene on complex properties and so do not require a distinct ontological category; two objects are members of the same kind if they supervene on the same conjunctive universals. He takes properties and relations rather than natural kinds to mark out the fundamental joints of nature for two reasons.

Firstly he questions whether there exist appropriate candidates for universals for higher level kinds, for example, is there a universal 'humanity' which every human instantiates? Since Armstrong wants to be naturalist, the property responsible for humanness must be biological. Potentially human DNA structure might be sufficiently abstract to serve as a sufficient and necessary condition for humanity but this causes another problem to arise. We may only treat this structure as a universal if it plays a non-reducible causal role. It must not be the case that the work required in maintaining a human being is actually performed by the constituent molecules in virtue of their determinate properties rather than the specified universal. It is not clear that this condition is met (Armstrong, 1997, 66).

Secondly Armstrong argues that even the most promising candidates for kinds can be given a reductive analysis suggesting that the electron can be reduced to the conjunction of the three properties; mass, charge and spin. He admits that

kinds like the electron mark out true (non-fundamental) joints in nature but claims this is insufficient to warrant a distinct ontological category. If kinds supervene on properties then whether or not they cut nature at its joints they are no addition in being (Armstrong, 1997, 67).

## 1:5:2: Ellis' Scientific Essentialism

Ellis rejects Lewis' and Armstrong's categorical monism according to which all fundamental sparse properties are categorical. However Ellis also rejects dispositional monism in favour of dispositional essentialism. Dispositional essentialism is the view that at least some properties have dispositional essences. Dispositional monism is the view that at least all sparse properties are essentially dispositional. A dispositional property is characterized by the fact that it is essential to the property that it manifests itself appropriately in the presence of a certain stimulus. A categorical property lacks this modal character; 'it does not confer of necessity any power or disposition… it has no necessary connections with any other entities' (Bird, 2007, 67). As I shall explore, Ellis prefers a mixed view which is equally committed to dispositional and categorical properties.

Contrary to Lewis and Armstrong, Ellis takes kinds to be more fundamental than particulars. He also argues that laws of nature are metaphysically necessary. He distinguishes between individual essences and kind essences. The individual essence of a thing is the set of the characteristics in virtue of which it is the individual it is, while the kind essence of a thing is the set of properties in virtue of which it is a thing of a kind it is (Ellis, 2002, 5). He argues for the existence of three hierarchies of natural kinds; substantive kinds instanced by kinds of object, dynamic kinds instanced by kinds of events or processes and finally property kinds instanced by tropes. Ellis takes kinds to be universals in the Aristotelian sense requiring instantiation in a particular for existence.

Interestingly for the purposes of my thesis, Ellis motivates his metaphysical framework with a discussion of chemistry. He focuses on chemical entities which he

claims are the paradigmatic examples of natural kinds and notes that they are each real and absolute; they constitute genuine categories in nature and as such do not depend on human interests. Each element is categorically distinct from every other – there are no non-arbitrary boundaries between different kinds and so there is always a fact of the matter whether a particular is a member of any given kind. In addition, it is in virtue of the possession of essential properties that an object is a member of a natural kind where essential properties are always intrinsic and are either categorical or dispositional. He states that if a particular belongs to two different natural kinds then the two kinds must be species of one common genus, i.e. two distinct natural kinds cannot overlap, rather one kind must include the other; this is referred to as the speciation requirement. Similarly, kinds form hierarchies such that the kind electron falls under the kind lepton which in turn falls under the kind fundamental property. Taken together these features constitute the conditions for natural kind hood for all three types of natural kind, according to Ellis.

Ellis also proposes a mixed view which retains the distinction between categorical and dispositional properties and takes them to be equally fundamental (Ellis, 2001, 127). Categorical properties are those that are had by things independently of how they are disposed to behave; shape and size are common examples. Dispositional properties on the other hand are those properties whose manifestation produces a kind of behaviour such as toxicity or fragility. As a result their identity <C, E> depends on the circumstances in which they would be displayed (C) and the form this manifestation would take (E), (Ellis, 2002, 117). Dispositional properties are crucial to Ellis's account since they do crucial work in unifying the three distinct hierarchies.

Ellis gives two reasons why categorical properties cannot be reduced to dispositional properties. In the first place he discusses block structural properties; these are properties that consist of relations between things which have independent identities. A molecule $CO_2$ is an example of a block structure since it exists if and only if the relevant constituent parts exist and are related in the correct way (Ellis, 2002, 69). Ellis maintains that this is evidence in favour of a categorical -

dispositional distinction, on the grounds that 'block structural properties are clearly not just dispositional' (Ellis, 2002, 69). Even if we learn about its structural properties via its dispositional properties, Ellis claims its essence is structural (categorical) and not dispositional (Ellis, 2002, 70).

Ellis also refers to the existence of intrinsic structures in order to support the distinction. Intrinsic structures are those in which the constituent parts cannot exist independently of the structure, so for instance the electric and magnetic potentials cannot exist independently of an electromagnetic field. Ellis maintains that these are structural properties; they might be dispositional structures but their essence is structural rather than dispositional (Ellis, 2002, 71).

Dispositional properties are central to Ellis's account since they do the work of unifying the three hierarchies. Firstly they constitute a generic category in the property kind hierarchy so Ellis is committed to the dispositional property kind as a kind in its own right. Secondly, dispositional properties constitute the essential properties of substantive kinds alongside categorical properties. Thirdly, Ellis takes a particular process kind to be the manifestation of a certain dispositional property; therefore processes that are members of the same process natural kind are instantiations of the same dispositional property (Ellis, 2001, 77). Ellis describes the essential nature of a process by referring to 'a structure that distinguishes it from all other kinds of process and in virtue of which it is a process of the kind it is. This is usually indicated by the chemical reaction that is used to describe the reaction' (Ellis, 2002, 33).

Ellis describes the relationship between dispositions, dispositional properties and causal processes as follows. Salt has the dispositional property 'solubility,' the manifestation of this property is the natural kind process, dissolution. The essence of the process can be given a description in terms of its structure i.e. the breakdown of the crystalline structure of salt due to interaction with a polar solvent. Any process that exhibited this essential structure would qualify as member of the natural kind dissolution. Any object that is capable of undergoing dissolution must possess the dispositional property 'solubility' (Ellis, 2002, 125).

He argues that the laws of nature that hold over a particular kind hold in virtue of the dispositional properties that are essential to that kind. In this sense natural kinds are more fundamental than laws of nature and in disciplines in which there are no natural kinds, there can be no laws of nature. To take an example, an essential property of the electron is the disposition to repel negatively charged things, consequently it is a law of nature that electrons repel negatively charged things (Ellis, 2002, 82).

A consequence of this account of laws is that laws are metaphysically necessary. This doesn't mean that in every possible world there exists the same laws of nature rather any two worlds that contain the same natural kinds will contain the same laws of nature. Since laws follow from essential properties it is metaphysically impossible, for instance, for an electron to not repel other electrons. It is an essential property of an electron that it is disposed to repel negatively charged objects; if it did not do so then it would fail to qualify as a member of the natural kind electron.

Since laws of nature hold in virtue of kinds there must be a natural laws structure that parallels the natural kind structure already in place and we should expect three hierarchies of laws of nature where more specific laws supervene on more general laws (Ellis, 2002, 85). This can be illustrated with reference to the dynamic kind hierarchy; at the highest level of generality are those laws that cover all kinds that fall within the hierarchy, these laws follow from the essence of the global process kind which is found at the top of the hierarchy. Further down the hierarchy we find laws of medium generality, these govern 'ubiquitous but not all natural kinds of process' and are entailed by the essential properties of generic kinds. Finally there exist laws that govern specific kinds of process only (Ellis, 2002, 86). The same model applies to substantive natural kinds but not to the property natural kind hierarchy - in this case Ellis admits that there is no global law that governs all kinds of properties; he takes this to be a potential argument for splitting the property hierarchy into two distinct categories; dispositional and structural properties (Ellis, 2002, 87).

### 1:5:3: Scientific Essentialism and Classifying Reactions

Ellis's account stays true to the naturalistic spirit in the sense that he notes that laws of nature refer to processes and on this basis builds a place for them in his ontology. However his response of committing to natural kinds of entities, properties and processes results in a significantly inflated ontology. Part of my task in the following chapters will be to examine whether this move made by Ellis is necessary to capture the classification of reactions. Alternatively, can this be achieved at a lower ontological price?

A further question for his account concerns how to flesh out his notion of a natural kind hierarchy. He equates the manifestation of a dispositional property with a kind of process where this process can be identified with a particular structure. In *The Metaphysics for Scientific Realism* Ellis expands on his discussion of the structure of processes and describes how this could be specified in the case of simple processes that fall at the bottom of the process hierarchy such as radioactive decay, particle emissions, absorptions or annihilations. He describes an 'elementary causal process' as an emission event, followed by a Schrödinger wave transmission process, followed by an absorption event (Ellis, 2010, 83-7).

As Chakravartty has pointed out this suggests an acceptance of the Salmon-Dowe model of a causal process in which processes are defined in terms of the transmission of conserved quantity where the details of what this quantity amounts to are provided by physics. Salmon tells us we have reason to believe that mass, energy and charge are conserved quantities. Chakravartty has suggested that thinking about processes in terms of fundamental physical properties is insufficient to capture higher level processes (Chakravartty, 2007, 158). In the case of the classification of reactions it is not clear that such an approach could capture the appropriate similarity relations between higher level reactions. For example, could the transfer of conserved quantities capture what is similar between two oxidation reactions and why this is different to a hydrolysis reaction? Even if we were to find alternative means of specifying the structure of higher level processes like reactions

by appealing to the structure of the reaction mechanism, again, it is unclear how much structural similarity is required for two reactions to be of the same kind.

Ellis' use of energy transfer to identify a process marks a different approach to that specified in the previous section in which reactions are identified in terms of a mechanism. My project in the forthcoming chapters will be to examine how we determine which of these is most appropriate to chemical practice. I'll show that both an appeal to causal structure as well as conserved quantities referred to by Salmon are relevant to this task.

## 1.6: Quine's Weak Realism

### 1:6:1: Thesis and Motivation

Quine is realist about natural kinds in the sense that he equates them with sets of entities and takes the concept of kindhood to be intimately related to the notion of projectability (Quine, 1969). He introduces kinds in order to account for two paradoxes of confirmation; Hempel's Raven Paradox and Goodman's New Riddle of Induction.

The ravens' paradox arises when we accept two plausible claims;

a. Positive instances of a generalisation provide confirming support for that generalisation
b. Something which confirms a generalisation also confirms any statement that is logically equivalent to that generalisation

By the first claim a black raven confirms the hypothesis that all ravens are black. The statement all ravens are black is logically equivalent to the statement that all non-black things are non-ravens which in turn is confirmed by a white shoe. However anything that confirms the latter statement must confirm the former since they are logically equivalent and thus we get the paradoxical conclusion that the statement 'all ravens are black' is confirmed by a white shoe (Hempel, 1945).

Goodman's new riddle of induction also gives counter intuitive conclusions with regards to confirmation. The predicate 'grue' is assigned to anything that is green and observed before now or blue and unobserved. If it's the case that all emeralds that have been observed so far have been green then they must also have been grue and so provide confirmation for the statement that 'all emeralds are grue'. In addition, if we combine this with the assumption that some emeralds are as yet unobserved then we get the paradoxical conclusion that some emeralds are blue (Goodman, 1983).

Quine attempts to dissolve the paradox by claiming that only natural kind terms are projectable. It follows from this that it is illegitimate to make projections based on the terms 'non raven' and 'grue' since they are not natural kinds. Consequently, whilst we might accept a black raven as a confirming instance of all ravens are black we cannot do the same for white shoe, nor can be make projectable judgements about 'grue' (Quine 1969, 116)

For Quine, kinds are sets whose members bear a similarity relation to each other (Quine 1969, 135). He admits that kindhood and similarity amount to the same notion but doesn't give an account of one in terms of the other. Instead, he denies that it is the job of the philosopher to define what is meant by kindhood rather he outsources the job to the particular branch of science to which the kind term is relevant. He suggests that different branches of science require different notions of similarity which are more or less fine grained and that it is a mark of a mature science that it has a well fleshed out notion of similarity. In addition, once a given branch of science has reached full maturity then it must be integrated into our current systematisation of nature such that the similarity notions advocated by different branches are compatible with each other. He argues that once this is achieved then the notion of kindhood and similarity are dissolved.

### 1:6:2: Quine and Classifying Reactions

Quine doesn't explicitly discuss the possibility of natural kinds of change however his arguments can be extended. If kinds are sets who members bear a similarity relation to each other then there is no reason why we can't have sets containing instances of chemical reactions each of whom proceeds in the same way, perhaps by the same mechanism.

Quine maintains that kinds are sets where members share at least one natural property. For example, Quine takes the set of positively charged objects to form a natural kind where this contains a hydrogen ion, an up quark and a charged water droplet. In the case of the classification of reactions sets containing chemical reactions would take a variety of different forms. For example, there is the set of all chemical reactions containing a carbon atoms or the set of all reactions containing an alcohol. Alternatively, if we return to the types chemical reactions outlined in section 1.2. we might identify the set of all chemical reactions involving the decomposition of a chemical entity into two or more substances via the breaking of the bond. If Quine's account of natural kinds is to apply to chemical reactions in a chemically accurate way then we may need to address whether particular commonly instanced rearrangements of atoms of bonds fall within his notion of having a natural property in common? Alternatively do we need to extend this discussion to natural properties and relations?

## 1:7: Boyd's Homeostatic Property Cluster Account

### 1:7:1: Thesis and Motivation

Boyd advocates the homeostatic property cluster (HPC) account. He is realist about natural kinds and takes them to be co-occurring clusters of properties that repeatedly co-occur due to the presence of an underlying causal mechanism or by homeostasis i.e. the presence of a property which favours the presence of other properties.

Boyd's realism about natural kinds is motivated by the role they play in our epistemic practice. He highlights this in his accommodation thesis which states that 'the theory of natural kinds is about how schemes of classification contribute to the formulation and identification of projectable hypotheses' (Boyd 1991, 147). He argues that scientists are typically successful in making inductive inferences and the best explanation of this success is that they have uncovered those taxonomical divisions that genuinely latch on to the causal structure of the world. Those homeostatic property clusters that continually co-occur and support inductive inferences give us reason to believe that they latch on to this causal structure. This allows us to make sense of the metaphor that 'kinds cut nature at its joints.' 'Kinds useful for induction or explanation must always "cut the world at its joints" in this sense: successful induction and explanation always require that we accommodate our categories to the causal structure of the world' (Boyd 1991, 139).

The accommodation thesis has been proposed as a potential line of attack in response to the inductive sceptic. If certain clusters of properties continually co-occur then we can infer from the presence of one property to the potential existence of another. Consequently, if it is the case that every F we have ever observed has been a G then it might be argued that the best explanation of our observations of only Gs and Fs is that all Fs are Gs. This thought is that if a term is to have significant projectability then it should latch on to a cluster of properties that are correlated for good reason and not by accident. As a result we should want to identify a condition C that explains why all F's are G's. Boyd's account attempts to provide this.

On the HPC account properties co-occur as a result of homeostasis or a causal mechanism. In the first case the presence of some of the properties in F tends, under appropriate conditions, to favour the presence of the others. In the second case, there are underlying mechanisms or processes that tend to maintain the presence of the properties in F, or both (Boyd, 1999) Figure 1 illustrates some of the relations that might hold between a property cluster (P1…P5) and a mechanism x.

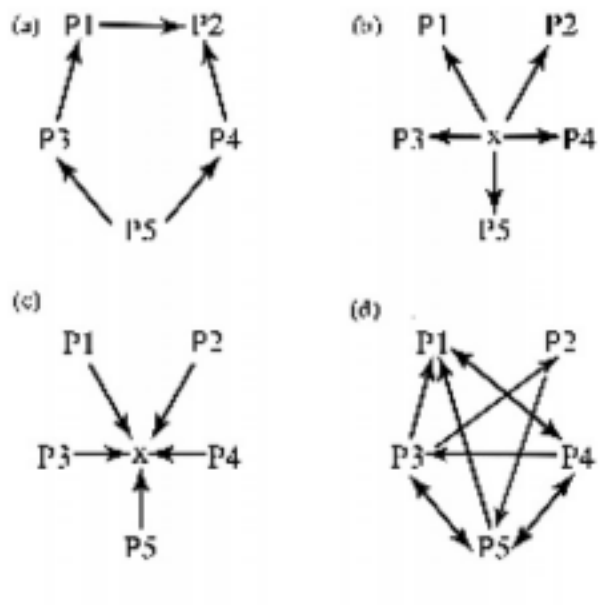


*Figure 1 Co-occurring clusters of properties resulting from homeostasis or a causal mechanism (Craver, 2006, 583)*

In examples a. and d. the clusters are self-sustaining; the presence of certain properties causes the presence of others. In case b. it is the presence of the mechanism x that causes the properties to co-occur, whilst in the example c. the cluster of properties gives rise to the mechanism.

Since not every property (P1…P5) must be instanced in order for the cluster to qualify as of a certain kind, in each instantiation of the mechanism there are no sufficient and necessary conditions on kind membership. Instead Boyd admits that cluster kind terms are often vague and there is no matter of fact about whether an individual falls within the extension of a term. The cluster of properties is assumed to have causal import; the co-occurrence of a number of the properties results in some significant effect and as a result any attempt to further refine the cluster in order to remove the vagueness of the extension of the kind term obscures this effect. Nonetheless, Boyd argues that we should be guided by the success of our inductive practice and as a result the properties which constitute any kind as well as their relative importance are a posteriori concerns.

## 1:7:2: Homeostatic Property Cluster Kinds and Classifying Reactions

The HPC account of classification is of particular interest when investigating the classification of reactions. This is because my discussion at the start of this chapter indicates that the notion of a mechanism is central to the way reactions are classified. One option would be to equate the reaction mechanisms of the sort described in section 1.2 with the co-occurrence of chemical properties. In this sense reaction mechanisms might be thought to permit inductive inferences. Consider the hydrolysis reaction. The reaction can be described in terms of a reaction mechanism; it involves the decomposition of a substance as a result of a polar charge on a $H_2O$ molecule. Additional chemical groups involved in the reaction are labelled as R and $R_1$, the identity of these groups in not relevant to the overall reaction mechanism.


*Figure 2: Generalised mechanism for a hydrolysis reaction*

Hydrolysis reactions which act on similar types of entities will result in similar product entities where these products also have similar properties. In this sense, reactions acting as causal mechanisms might be thought to produce co-occurring clusters of properties.

One option for developing the HPC account is to reconcile Boyd's use of the term 'mechanism' with the recent literature on mechanisms. Craver (2009) investigated this approach and uncovered difficulties for the HPC account. He concluded that the HPC account is not the middle way between conventionalism and essentialism that Boyd hopes.

Craver's argument is that conventional elements are involved 'partly but ineliminably' in deciding when two mechanisms are of the same type and secondly, when identifying when one mechanism ends and the other begins (Craver, 2009, 575). For Boyd, two clusters are of the same kind if they are produced by the same

mechanism and therefore Craver argues that these considerations affect which properties constitute any given cluster.

Craver's arguments rest on the claim that there are many different and contradictory ways in which we might choose classify mechanisms together depending on our pragmatic interests. Craver states; 'if the HPC account were to suggest that we should split kinds whenever the mechanisms differ in any of the myriad ways that any two mechanisms might differ then there would be as many kinds of mechanisms as instances of mechanisms' (Craver, 2009, 579). He suggests that Boyd would want to avoid this conclusion yet, at the same time there appears to be no fact of the matter when a sufficient degree of similarity holds between two mechanisms for them to be of the same kind, thus according to Craver, Boyd's account edges towards constructivism (Craver, 2009, 579).

However, Craver's objection fails to acknowledge the central role in identifying stability in Boyd's account. Consequently, rather than trying to isolate a particular mechanism and then reading off the properties that would form a natural kind as a result as Craver suggests, Boyd's account employs the reverse approach. Boyd first isolates co-occurring properties and then seeks to uncover the homeostatic mechanism responsible. Boyd also accepts that HPC kinds are discipline relative and admits that 'natural kinds for psychology may turn out to not be natural kinds in the same sense for physiology' (Boyd, 1999 145). As a result, Boyd would not accept that the tension which Craver is alluding to is problematic.

It is also worth noting that Boyd says very little about the nature of a mechanism. This is in spite of the fact that in at least some cases, it is the homeostasis or a causal mechanism that has ontological priority in that it produces the clusters of properties required for projectability. In addition, Boyd does not discuss the possibility of kinds of process. I suggest Boyd's account might be a fruitful avenue of inquiry for the classification of reactions. I will return to this point in chapter 3 and again in chapter 6.

# 1:8: Dupré's Promiscuous Realism

## 1:8:1: Thesis and Motivation

Dupré's promiscuous realism advocates a pluralist and weakly realist conception of natural kinds in which a best or correct classificatory system exists only with respect to a specific scientific interest. The motivation for Dupré's promiscuous realism is classificatory practice in biology. One of the questions he is interested in concerns what criteria should be used when determining species membership. He argues that this question has no definite answer and instead identifies three plausible candidates for the essential property of a species. (Dupré, 1981, 80 – 90)

1. The phylogenetic conception of species states that a genetic description could function as the essential property of a species such that members of a species share some genetic blue print where physiological and morphological differences result from the interaction between the organism's genetic makeup and the environment. The problem with this approach is that members of the same species tend to exhibit a high level of genetic variability, and for good reason since this trait is favoured by evolution on the grounds that it increases the ability to adapt to a changing environment (Dupré, 1981, 87).
2. The second potential criterion for species membership is reproductive isolation. On this account a species is defined as a group of interbreeding individuals. This criterion is also inappropriate to some cases as a result of hybridization which frequently occurs in the natural world. In the case in which the hybrid is infertile we are left with an individual that is not assigned to any species. In the cases in which reproduction is possible the 'alien' genes are not competitive enough to survive further rounds of reproduction and we are still left with reproductive links between distinct species, discrediting the criteria (Dupré, 1981, 85).

3. The third criterion is concerned with evolutionary history. It is assumed that if it was possible to construct a family tree beginning from the start of life we

could state that something is a member of a species if it has the correct ancestry. This option is problematic because a completed ancestry tree is impossible to produce; evidence left by organisms in the very distant past is no longer available (Dupré, 1981, 87).

Dupré argues that because of the difficulties with each of the definitions we should concede that there is no single definition of a species rather biologists choose to use one of the above depending on what they are interested in. It is this ability to read off different philosophical conclusions directly from scientific practice that convinces him that essentialism is false and that inspires promiscuous realism (Dupré, 2002, 38).

Dupré denies that there is a unique set of natural kinds that results from an ultimate classificatory system. However, he insists that the different classificatory systems which arise out of different research interests are equally real. He considers kinds to be a useful methodological tool on the grounds that it is the application of theoretical concepts that divides nature into groups (Dupré, 2002, 39). Dupré states explicitly that the process of sorting nature into kinds and deciding which concepts are relevant for classificatory purposes are two sides of the same coin (Dupré, 2002, 45).

Nonetheless Dupré does take classification to be constrained by nature. The aims of a particular inquiry are a matter of historical contingency which means that the outcome of scientific inquiry is not necessarily determined in advance even if we are realist about modes of classification. He is however, open to the possibility that 'all paths lead to Rome' and that certain scientific doctrines are inescapable regardless of our specific goals of inquiry (Dupré, 2002, 47).

Dupré is a weak realist about kinds and he rejects any metaphysical account of kinds. He does not distinguish between knowing the essence of an individual and knowing the natural kind to which it belongs, rather, once we know what the natural kind is we know what the essence is, this is what Dupré calls a 'bare essence' (Dupré,

2002, 44). On this conception of natural kinds it makes no sense to ask what the essential property of a particular is.

## 1:8:2 Promiscuous Realism and Classifying Reactions

In his most recent book *The Processes of Life 2012* Dupré extends these themes. He advocates Promiscuous Individualism the idea that organisms are constituted by processes rather than entities; 'Key concepts in biology, I suggested, are static abstractions from life processes, and different abstractions provide different perspectives on these processes' (Dupré, 2012, 86).

This view provides the metaphysical accompaniment to promiscuous realism. Dupré defines a process as 'anything that must continually undergo change in order to survive,' and describes how scientists abstract entities away from processes in those places where processes give the illusion of stability (Dupré, 2012, 86). Scientists working at different levels will identify different instances of stability according to their research interests and so will identify different particulars each of which has the potential to contradict each other.

The priority of processes over entities has the implication that there is no unique answer to questions regarding how many organisms are present in a given system. Dupré states that 'what an organism is, and whether something is part of an organism or not, are not questions that necessarily admit of definitive answers' (Dupré, 2012, 153). This can be fleshed out using the biological example of lichens which are composite organisms consisting of a symbiotic relationships between a fungus and a photosynthetic partner which is usually a green algae. (Dupré, 2012, 158).

Dupré challenges the view that there is one organism present, the lichen, or two organisms present, the fungus and algae. Rather, he claims there are three organisms; the lichen, the fungus and the algae and we prioritize one answer over the others depending on our interests. In addition, the fungi that jointly constitute the lichen consist of millions of cyanobacteria, and there are multiple ways in which

we can draw the boundaries between an individual fungus of a given species, with the consequences that individuating particulars gives rise to high levels of promiscuity (Dupré, 2012, 158).

By reversing the traditional priority relation between entities and processes Dupré has outlined a metaphysical framework for his promiscuous realism. Different and contradictory classificatory schemes arise when the illusion of stability is identified from different perspectives. Whilst Dupré is concerned with classification in general and also with the status of entities he does not address the classification of processes or commit to natural kinds of processes. He has not addressed the classification of chemical reactions.

I suggest that his definition of a process is vague; he states only that a process is something that must continue to change in order to continue to exist. This isn't useful for my purposes since it provides little clue about how we should distinguish one kind of process from another, e.g. a hydrolysis reaction from a substitution reaction. Perhaps, however, his definition of a process can be extended in such a way that might shed light on the nature of a chemical reaction. I will return to this point in chapter 4.4 and offer my own definition of a process.

## 1:9: Chemistry in Context: Microstructuralism

So far in this chapter I have addressed general debates about classification in the philosophy of science. Chemistry has always been central to debates about classification. However, as I discussed at the start of my thesis, the past 20 years has seen the birth of the philosophy of chemistry in its own right and this has implications for our understanding of classification. In particular philosophers have attempted to produce a chemically informed understanding of classification that is compatible with more advanced chemical knowledge. In the following section I will outline a specific debate within the context of the philosophy of chemistry between microstructuralists about chemical classification on the one hand and those that advocate a thermodynamic approach to classification.

### 1.9.1: Thesis and Motivation

Microstructuralism about chemical kinds is advocated by Hendry (2006) and is the thesis that membership of a kind is conferred by microstructural properties. The paradigmatic examples are provided by the chemical elements in which the relevant microstructural properties are the number of electrons in the outer shell, or in the case of isotopes, the number of neutrons present in the nucleus. On Hendry's view microstructural properties determine the extension of the kind but he stops short of full essentialism and doesn't commit to the idea that kinds have microstructural essences.

Hendry's motivations are twofold. In the first place, he appeals to the kind of modal intuitions advanced by Kripke. Hendry asks us to imagine a possible world in which water has different macroscopic properties such as a different boiling point or density and argues that this is conceivable. He then asks us to imagine another possible world in which water exists but is not formed from $H_2O$ molecules, he argues that this is impossible and that as a result being $H_2O$ is a necessary if not sufficient condition on being water (Hendry, forthcoming).

Secondly, Hendry is motivated by the idea that structure plays an important regulatory role with respect to the non-structural properties of the entity. In the case of the molecule ethene which consists of two carbon atoms joined by a double bond, Hendry argues that the presence of the double bond between the carbon atoms is a structural property (Hendry, forthcoming). As a result the presence of a high electron density and the ability to undergo certain types of reactions supervenes on a structural property in his view.

Hendry doesn't commit to microstructural essence for good chemical reasons. Once the level of complexity is increased microstructuralism becomes more complicated and vagueness enters the picture. At the level of the compound specifying, only the constituent parts of the entity becomes insufficient for distinguishing the extensions of what we intuitively consider different kinds. Consider the two distinct chemical substances ethanol and methoxymethane, they are

isomers; consisting of the same components in the same proportions, 2 carbon atoms, 7 hydrogen atoms and an oxygen atom. The difference between the hydrocarbons is due to the differing arrangements of the atoms in the compounds which are captured by the formulas $CH_3OCH_3$ for methoxymethane and $CH_3CHOH$ for ethanol. As Hendry points out 'the distinctness of ethanol and methoxymethane must lie in their molecular structures' (Hendry, 2006, 871). Therefore the different properties possessed by the two entities must, according to Hendry, supervene on spatial arrangement.

A consequence of extending the notion of microstructural properties to include a reference to spatial arrangement is that molecular structure is defined in terms of factors such as inter nuclear distances and angles between bonds, both of which are continuous variables. Consequently the similarity of one molecular arrangement to another is not a binary matter but a matter of degree. This means that chemical kinds cannot be divided into 'mutually exclusive and jointly exhaustive extensions' (Hendry, 2006, 871) Instead, they will form overlapping clusters of similar entities that are identified by the equilibrium point of the cluster but have no definite boundaries between the extension of one kind and another. However, since Hendry is not committed to the stronger essentialist claim that chemical kinds have a microstructural essence he can embrace this vagueness and accept that the extensions of complex chemical kinds do not have definite boundaries (Hendry, 2008, 115).

### 1.9.2: Microstructuralism and Classifying Reactions

Hendry does not explicitly discuss the classification of reactions. He states only that entities provide the ingredients of reactions and provides an analogy with baking a cake and suggests the atoms and bonds which undergo a reaction are used up in the reaction process just as ingredients are used up in a cake (Hendry & Needham, 2011).

A further way to address whether microstructuralism can capture the classification of chemical reactions is to examine the position in light of the criticisms levelled against it. Much of the discussion between microstructuralism and its opponents takes place within the context of the question, 'is water $H_2O$'? Needham and van Brakel suggest that an account of a complex substance like water requires reference to macroscopic as well as microstructural properties (Needham, 2000) (van Brakel, 2000). They claim that it is misleading to assert that 'water = $H_2O$' on the grounds that water cannot be equated with a single $H_2O$ molecule since this molecule would lack the stereotypical features associated with water. It wouldn't have a boiling point, temperature or thirst quenching ability. Even if we employed a modified reading of the identity statement so that it read 'water is a collection of $H_2O$ molecules' it would still not do the job of accounting for the behavioural properties of water according to Needham (Needham, 2011). These properties are accounted for not by the structure of a $H_2O$ molecule but by the higher level thermodynamic properties of water.

Needham and van Brakel draw our attention to the fact that paradigmatic samples of water contain significant amounts of impurities but the $H_2O$ molecules themselves present in solution are constantly disassociating and then re-associating according to the following equilibrium $2\ H_2O \leftrightarrow H_3O^+ + OH^-$ (van Brakel, 1986) (Needham, 2010.) In addition those $H_2O$ molecules that are not disassociated at any one time possess a polar charge which causes them to undergo intra molecular bonding and form oligomolecular species or long chains of $H_2O$. These chains are constantly breaking and reforming as $H_2O$ molecules continue to dissociate. Needham and van Brakel assert that it is this thermodynamic picture that is responsible for the stereotypical properties of water rather than an individual $H_2O$ molecule.

In order to assess whether microstructuralism adequately captures the classification of chemical reactions I must assess whether the same worries about the need to capture the thermodynamic properties of entities also apply to reactions. Are all the characteristics of reactions that are relevant to chemical understanding

captured by a microstructuralist account? I will address this debate in section 2.3.2 where I argue that when classifying chemical reactions, chemists attempt to explain macroscopic differences at the microstructural level. Therefore it is the unification of microstructural and macroscopic properties that is important to chemical practice. I will further discuss thermodynamic understanding of reactions in section 4.4.

## 1:10: Conclusion

In this chapter I have introduced the notion of a chemical reaction and the intuition that reactions can be classified into types. I introduced key accounts of classification from social constructivism, semantic essentialism, metaphysical essentialism and the weaker realist positions about classification.

I suggested that many of the traditional accounts of classification do not address the classification of non-entities like things such as reactions. Expanding any of these accounts to accommodate the classification of reactions will require answering some key questions. The first concerns the status of reaction classifications; are they of the same status as classifications of entities? In other words do classifications of reactions cut nature at its joints or support law like generalisations in the way that some philosophers argue that entity classifications do?

A further question concerns the way in which reactions are classified. In chemical practice are sufficient and necessary conditions for kind membership specified and if so on what basis? One option is to individuate reactions using the causal structure of reactions and another is to appeal to a conserved quantity approach. In both cases the classification must be able to capture fine and coarse grained similarities between the different reactions. For example, the kind 'oxidation reaction' contains coarse grained similarities as it permits a high degree of lower level variation. The kind 'photosynthesis' captures more fine grained similarities as there is less variation between token instances of the kind.

It should also be noted that the different accounts appeal to different ontological resources. Ellis commits to a natural kind category of processes, whilst Dupré offers a very different account in which processes are treated as prior to entities.

Boyd on the other hand commits to mechanisms to sustain his account, which is in contrast to Hendry who commits only to microstructural properties. A key part of my project of deciding which, if any, of the accounts of natural kind classification is most appropriate to reactions, will involve evaluating which ontological components are necessary for classifying reactions. In chapter 2 I will discuss the classification of reactions in practice and outline a framework of criteria by which to evaluate which ontological components are required. I will argue at the end of chapter 2 that there is good reason when assessing the classification of reactions in practice to begin by looking to the mechanisms literature in chapter 3. The results of this discussion will point me towards and assessment of the entities – dispositions ontology in chapter 4 and causal dispositionalism in chapter 5. In chapter 6 I will outline a positive proposal for a metaphysics of the classification of chemical reactions in practice.

# Chapter 2: Classifying Reactions in Practice

## 2.1: Introduction

My aim in chapter 1 was to give an overview of the debate on the status of the classification of scientific entities. I provided an introduction to the notion of a chemical reaction and showed that a brief survey into chemistry reveals that chemists classify reactions into types and tokens in addition to the more familiar classification of entities into types and tokens. I outlined different philosophical approaches to classification from constructivism to essentialism about natural kinds and the weaker realist positions that fall in between. I concluded that none of the positions outlined in chapter 1 can straightforwardly accommodate the classification of chemical reactions without further development. This is because with the exception of Ellis's *Scientific Essentialism* the different philosophical accounts are primarily concerned with the classification of entities and further work is done to show how they might accommodate reaction classification, if this is indeed possible. With respect to Brian Ellis's Scientific Essentialism, while he does discuss the classification of reactions and make room for natural kinds of reactions in his ontology, he does not argue for this conclusion using a detailed consideration of scientific practice. My methodology, in contrast to Ellis', is to give an account of the classification of reactions that is purposely led by scientific practice, I shall discuss this in detail in sections 2.3 and 2.5 of this chapter.

In order to establish which philosophical account of classification is most appropriate for chemical reactions it is necessary to further explore how the classification of chemical reactions is achieved in chemical practice. My aim in this chapter is to build a picture of the classification procedure, including the aims and objectives of the classification, the details of how the classification takes place and

how the output classification is received and absorbed into chemical knowledge. I will then draw together this discussion to provide a list of criteria and requirements that any metaphysics of classification must adhere to if it is to accommodate the classification of chemical reactions in practice.

One of the implications of this chapter is that the discussion will enable me to answer some of the questions raised in chapter 1. For example, we know that reactions are classified into types but does this always happen on the basis of the underlying reaction mechanisms such as addition, elimination, substitution and combination? Is it the case that the structure of the reaction mechanism provides the essential properties on which reaction classification is based? If this is the case then how do chemists manage the role played by structure and the potential for vagueness that is described by Craver and discussed in chapter 1? If it is not the structure of the reaction mechanism then what provides the conditions for kind membership?

I'm also interested in the aims and interests of chemists when they produce classifications. For instance, are they used to support predictions and the fruitful development of science? Alternatively, are they employed for the purpose of storage or to effectively convey information to students of chemistry? Addressing these questions will provide a preliminary basis for adjudicating which general account of classification, if any, is most appropriate, whether this be constructivism, realism or essentialism.

I will begin in section 1 by outlining the chemical context in which my discussion will take place, focusing specifically on the domain of chemoinformatics. In section 2, I'll discuss a new approach to classifying reactions and its first application on a test case of common organic reactions which were classified to demonstrate the effectiveness of the new methodology. In section 3, I use this methodology to draw out three initial requirements that a metaphysics for the classification of reactions must be compatible with. These initial requirements are related to the details of the three stage classificatory process; the use of reactions as a heuristic device to guide classification, the application of QSAR and the application of neural networking.

In section 4 I describe a more recent case study in which this same methodology is applied to the classification of reactions with the aim of enhancing predictability and advancing chemical knowledge. This discussion allows me to draw out three more general constraints on a metaphysics for the classification of reactions, by meeting these criteria an ontology is descriptively fit for purpose. In order to be descriptively fit for purpose it must be descriptively accurate enough, capture objective similarities and drive explanatory unification. These criteria will provide a way of adjudicating between the different metaphysical accounts of classification that are discussed through the course of my thesis.

My discussion of chemical practice will focus on the field of chemoinformatics, a relatively new sub-discipline within the field of chemistry that began to emerge in the 1980s. The remit of chemoinformatics is the '*application of informatics methods to solve chemical problems'* and the field covers three areas; data management, learning and representation (Gasteiger, 2001, 1)[5]. My thesis will focus on the application of informatics techniques to achieve chemical learning although questions of data management will be relevant at times. The aim of chemoinformatics with respect to my case studies is to use empirical data to solve chemical problems by employing different learning techniques.

The two main types of learning employed in chemoinformatics are deductive learning and inductive learning. In order to proceed by deductive learning you chemists require a fundamental theory from which you can base inferences and predictions. Quantum mechanics is the best fundamental theory available for chemistry. The Schrödinger equation can for example, be used to establish the

[5] Data management involves the storage of huge and increasing amounts of data in chemical databases which are accessed electronically. Basic database theory has been developed to aid the tagging of data and to develop search and retrieval methods to ensure databases queries are dealt with as efficiently as possible (Gasteiger, 2003, 274)
Representation involves the representation of chemical compounds in their molecular structure and the representation of chemical reactions. My thesis will not focus on the role of representation of distinct entities however I will address the representation of similarity relations holding between the objects of investigation, in section 2.2.2

dependence of the properties of simple molecules on their three dimensional structure thus allowing for the calculation of their properties.

However, for complex molecules the application of the Schrödinger equation is not possible due to either gaps in the underlying theory or the large amounts of computation time that is required (Gasteiger, 2003, 7). In the case of chemical reactions the situation is worse still; only simple reactions can be analysed using the Schrödinger equations as more complex reactions require a series of approximations that affect the accuracy of results. In addition chemists are currently unable to give a quantum mechanical account that takes into account reaction conditions such as solvents, temperature, pressure or catalysts (Gasteiger, 2003, 2).

Since many of the properties and activities that chemists need to predict are beyond the capabilities of deductive learning at this time, inductive learning techniques have been embraced. Inductive learning involves identifying correlations between chemical structures and their properties on the basis of empirical data. This information is then organised in a scheme that allows the features that the entities or reactions have in common to be recognised. A classification scheme is built on the basis of this and is used to make further predictions (Gasteiger, 2003, 9). As I shall go on to discuss, these predictions concern which entities will undergo which type of reactions, which enzymes will act as catalysts for which reactions and how much activation energy is required in each case.

This approach to classification was pioneered by Johann Gasteiger, the founding father of the chemoinformatics movement who received the Gmelin Beilstein medal from the German Chemical Society in recognition of his contribution to the field. My thesis will focus on the work of the Gasteiger research group based in Erlangen Nuremburg and their development and application of inductive learning techniques in order to further our understanding of chemical reactions. 'The automatic perception of chemical similarities between chemical reactions is required for a variety of applications in chemistry' (Latino and Aires de Sousa, 2011, 325). The techniques outlined in this chapter are now utilized worldwide in major industrial and academic research and discovery laboratories to design and optimize chemical

products and processes. In particular it supports the prediction of chemical, physical and biological properties of chemical compounds including their chemical reactivity and metabolic or environmental fate. This innovative approach has now become wide spread and is worthy of philosophical consideration. It is has become common place in domains such as Biochemistry for the Life Sciences (P, Atkins and de Paula. J) Molecular Informatics (Baumann, K. Ecker, G. Mestres, J. Schneider. G, 2014) Drug Design (Xu and Hagler, 2012) and Environmental Research (Devillers, 2014). Therefore there is reason to believe that the conclusions of my investigation will have a broader scope and be applicable to the philosophy of science more generally.

In this chapter I will discuss the application of inductive learning techniques to chemical reactions in the fields of organic chemistry and biochemistry. Each case study uses the same technique, the case study involving organic reactions is the first application of the technique in 1997 (Gasteiger and Chen, 1997). The second case study is a more recent application of the methodology from 2009 (Sacher, Reitz and Gasteiger, 2009). Both proceed by using inductive learning techniques to produce a classification of reactions that identify the similarity relations that hold between distinct reactions. In the first case these similarity relations are used to establish the reliability of the classification methodology by comparing the results to existing classifications. In the second case the classification was used to make predictions and support the fruitful development of science. The list of requirements that a metaphysics of classification must be compatible with if it is to accommodate chemical practice will be drawn directly from these case studies.

## 2:2: A New Methodology for the Classification of Organic Reactions

In the pioneering paper *Knowledge Discovery in Reaction Databases: Landscaping Organic Reactions by a Self-Organizing Neural Network* (Gasteiger and Chen, 1997), a new methodology for the classification of chemical reactions is outlined. Gasteiger explains that the approach is motivated by the way in which

chemists conceptualise chemical problems when faced with a small set of data and need to make predictions about reaction viability, products and yield.

> 'In most cases [chemists] solve these problems using something like a reaction map in their brain. Such a reaction map organizes reactions on the basis of chemical knowledge they have learned from textbooks and their experiments. So each chemist has her own reaction map' (Leach and Gillett, 2003, 1).

Gasteiger and Chen attempt to recreate the notion of a reaction map but on a scale beyond that of a single chemist thus requiring the application of informatics techniques. They described how they began their investigation by identifying the steps by which chemists build their own individual reaction maps;

1. Isolate and observe a phenomenon of interest

2. Analyse the factors that produce the phenomena using theoretical knowledge

3. Accumulate data on the factors that affect the phenomena of interest

4. Organise data systematically

5. Use statistical techniques to identify similarities between the phenomena of interest

6. Construct theories and laws governing the phenomena on the basis of these similarities

7. Use these theories to produce inductive inferences (Chen and Gasteiger, 2007, 4033).

Gasteiger and Chen's methodology mirrors this approach on a larger scale. The application of computational methods to the classification of chemical reactions means that an analysis of large volumes of data is now possible. They identified that;

> 'the number of observed reactions is extremely large and is increasing day by day. Some of them is published in articles and/or stored in databases on a

> computer. The number of the published and stored reactions goes into the millions. A reaction map in a brain of a chemist is constructed from only a part of these reactions, because anyone cannot see all of these reactions' (Gasteiger and Chen, 1998, 4033).

I will focus on two distinct methodological components that are required for the large scale classification of chemical reactions.

1. Application of QSAR (Quantitative Structure Activity Relations): the approach by which the relevant data for the classification of a particular phenomenon is identified
2. Application of neural networking: the process by which the data is manipulated to produce a two dimensional representation of the similarities that hold between reactions.

These two methodological components are applied together in order to produce a classification of reactions.

## 2:2:1: Part 1 and 2: Activities as Heuristics and QSAR

The aim of the search for Quantitative Structure Activity Relations or QSAR is to relate the observed chemical phenomena of interest to the underlying structural properties that correlate with the instantiation of that phenomenon. In discussion of chemical reactions, the term activity or A in QSAR refers to the instantiation of the reaction of interest.

> 'QSAR takes a series of chemicals and attempts to form a quantitative relationship between the biological or chemical effects (i.e. the activity) and the chemistry (i.e. the structure) of each of the chemicals, then we are able to form a quantitative structure–activity relationship or QSAR' (Gasteiger and Engel, 2008, 10).

The underlying belief or assumption is that lower level structural similarities give rise to similarities in higher level activities. Therefore once a relationship has been identified it provides the basis on which to make predictions about future occurrences of that activity, this assumption is that 'untested compounds possessing

similar molecular features as compounds used in the development of QSAR/QSPR models are likewise assumed to also possess similar activities' (Gasteige and Engel, 2008, 10).

The birth of QSAR can be traced back to France in the late 19th century. A paper entitled 'Action de l'acool amylique sur l'organisms by A. Cros described an empirical relationship between the toxicity of alcohols and the number of carbon atoms (Cros, 1863). This was followed in 1875 by Dujardin - Beaumetz and Audige who established the mathematical character of the relationship between the toxicity of alcohols and chain length and molecular structure (Dujardin - Beaumetz, and Audige, 1875, 192 – 194). In 1899 Hans Horst Meyer showed that narcosis or hypnotic activity has linked to the affinity of substances to water and lipid sites within the organism (Mayer, 1899, 109 – 118).

The birth of QSAR proper came in 1930 when Lazarev, a Russian chemist demonstrated that physiological and toxicological effects of molecules were correlated with the property of oil - water partition coefficient and that this could be demonstrated through a formal mathematical equation.

$$\text{Log } C = a \log K_{\text{Oil - water}} + b$$

where a and b are empirically derived constants and C is the molar concentration of the chemical. This physiological behaviour of the chemical was expressed as a function of its chemical constitution therefore any change in chemical constitution would be reflected in a corresponding effect on its biological properties. This equation can be considered the first general formulation of a quantitative structure – activity relationship (Consonni and R. Todeschini, 2010, 33). Since then QSAR has been a staple feature of chemoinformatics and has played a critical role in assessing the potential of new molecules for use in industry. More recently the application of QSAR to drug discovery has become increasingly important;

> 'The ability to predict a biological activity is valuable in any number of industries. Whilst some QSARs appear to be little more than academic studies, there are a large number of applications of these models within

industry, academia and governmental (regulatory) agencies. A small number of potential uses are listed below;

- The prediction of a variety of physicochemical properties of molecules (whether they be pharmaceuticals, pesticides, personal products, fine chemicals, etc.)
- The prediction of the fate of molecules which are released into the environment
- The rationalization and prediction of the combined effects of molecules
- The prediction of toxicity to environmental species
- The rational identification of new leads with pharmacological, biocidal or pesticidal activity' (Consonni and R. Todeschini, 2010, 4).

It is worth noting that in some of the chemoinformatics literature, reference is made to Quantitative Structural Property Relations (QSAP) alongside QSAR as discussed above. This suggests that a distinction may exist in the chemical literature between properties on the one hand and activities on the other. Such a distinction could have important implications for the metaphysics of classification, particularly if it turned out that an ontological distinction between properties and activities already exists in practice. It is asserted that 'QSPR methods are based on the hypothesis that changes in molecular structure are reflected in changes in observed macroscopic properties.' Examples of macroscopic properties are described as 'mechanical, thermal, electric etc.' (Consonni and R. Todeschini, 2010, 18).

This hints at a difference between the two domains such that QSPR allows chemists to predict that an entity has a certain property while QSAR allows chemists to predict that an entity will engage in certain activities. Nonetheless, there is no a discussion in the chemical literature on the difference between an activity and a macroscopic property and typically the terms QSPR and QSAR are equated. Part of the reason for this is that QSAR and QSPR tend to be used to refer to the methodology behind an investigation and this methodology is the same regardless of whether it is directed towards the study of activities or properties. For instance it is claimed that 'the first fundamental task in chemistry is to make inferences about which structure might have the desired property. This is the domain of establishing structure - property or structure activity - relations' (Gasteiger and Engel, 2008, 3).

The aim of my thesis is to give a metaphysics for the classification of reactions in practice. The case studies I discuss involving the classification of reactions refer only to QSAR and as result I will not make further reference to QSPR. This decision is not relevant to the arguments that follow in later chapters. In addition, in section 3.4 and 3.5, I discuss in detail whether the activities referred to in QSAR are philosophically speaking as, best construed properties or activities.

I shall now return to my first case study; the investigation into the classification of chemical reactions by *Gasteiger and Chen (1997).* QSAR was used to identify the structural properties that correlate with the instantiation of certain types of chemical reactions. The set of reactions to be classified and the corresponding data were taken from the ChemInform RX reaction database. This contains empirically derived information on 1.5 million reactions retrieved from publications appearing in the top 100 related journals from 1990 onwards (Gasteiger, 1994).

Gasteiger and Chen then narrowed down their test set of reactions to 120 reactions that involved the addition of a C-H bond to a C=C bond where this set was known prior to investigation to comprise a variety of distinct types of reactions (Gasteiger & Chen, 1998). This particular data set was chosen as it provided an appropriate test case. Gasteiger and Chen note that the sample size was manageable and there was a clear prior agreement on how the reactions should be classified so the success of the classificatory procedure was dependent on its ability to pick out these particular reaction types.

Gasteiger and Chen take the activity in question to be the instantiation of a particular known type of reaction, in this case the reaction is designated by the making and breaking of certain types of bonds. The structural properties specified by the 'S' in QSAR refer to properties of the reaction centre i.e. the properties of those atoms and bonds that undergo change during the reaction. It is thought that these features will be indicative of the type of change that will occur during the reaction. In later case studies chemists referred to reactions as being 'encoded by their structural properties' (Sacher, Reitz and Gasteiger, 2009, 1534).

The structural properties do not refer to the molecular geometry of the atoms and bonds specifically but are rather the physicochemical properties that affect molecular geometry such as charge distribution, inductive effect, resonance effect, polarizability effect etc. These properties are used because they provide the best indication of the mechanism by which each reaction will proceed. As previously mentioned this method is employed because quantum mechanical treatments of complex reactions are currently beyond our theoretical capabilities.

The exact physicochemical properties that best determine the course of any given reaction will vary case by case as identifying the correct properties is a matter of determining the structure-activity relation governing a particular reaction. In this case the six properties listed below were used. It was thought that reaction centres possessing similar values for the following variables were likely to undergo the same kind of organic reaction. Each reaction was assigned a value for each of the properties and these six values were taken as encoding each reaction.

1. Difference in partial atomic charges which describes the polarity of the bond

2. Difference in sigma electronegativities which describes the ability of an atom to attract electrons in a sigma bond[6]

3. Difference in pi electronegativities which describes the ability of an atom to attract electrons in a pi bond [7]

4. Effective bond polarizability which describes the tendency of the bond electrons to be distorted by an external electrical field

[6] A Sigma bond is the strongest type of covalent bond formed by a head on overlapping of atomic orbitals

[7] A Pi bond is a weaker form of covalent bind due to a reduced overlapping between the atomic orbitals

5. Delocalization stabilization of a negative charge on reaction centre which describes the stabilization of a negative charge generated by the heterolysis of the bond[8]

6. Delocalization stabilization of a positive charge on reaction centre which describes the stabilization of a positive charge generated by the heterolysis of the bond

Once a set of properties have been identified that are known to correlate with the particular activity of interest then the QSAR aspect of the classification procedure is complete.

## 2:2:2: Part 3: Neural Networking

The third part of the classification methodology involves organising the properties in a neural network in such a way to produce a representation of the similarities that hold between the reactions. Each reaction is encoded by values for each of these properties. The values for each reaction constitute a reaction vector that exists in a multi-dimensional space. In this case study, values for six properties were used for classification so the resultant vector exists in a six – dimensional space.

Gasteiger and Chen then employ a Kohonen network or a self-organising map that organises the vectors according to the similarity relations that hold between them thus resulting in a representation of this six dimensional space in a two dimensional plane. In this case all six values are weighted equally. The advantage of using a neural network is that the results are not skewed, if for example, the values of some properties contain low information or information of high redundancy with respect to other structural properties that are also included in the reaction vector. This is because in contrast to other methods of analysis, such as multi-linear regression analysis, neural networks are not sensitive to linear dependencies in the input variables. Gasteiger has described how 'this means that one can use all of the

[8] A heterolysis bond is one in which the process of breaking a covalent bind in which the shared electrons are claimed by one of the chemical species.

available physicochemical factors as input to the neural network; this both is simple and can avoid losing information' (Gasteiger, 1997, 4034).

Nonetheless using more input variables may require a significantly increased amount of time and resources but not produce any extra payoff in terms of the accuracy of the output classification. An offshoot of work into classification via neural networking are investigations into determining the optimum number of variables to be employed in a neural network.

The neural network works by preserving the topology of the original multi-dimensional space, therefore points that are close to each other in the six dimensional space will also be close to each other in the two dimensional representations The neural network consists of a cubic structure where the neurons are columns arranged in a two - dimensional system, e.g. in a square of n x 1 neurons. This is illustrated below in figure 3. The number of weights had by each neuron corresponds to the number of dimensions of the input data. In this case each neuron has six weights and in total there are 74 neurons corresponding to the number of reactions undergoing classification. Because of the relatively small number of reactions undergoing classification, chemists choose to operate with more neurons than required to allow for the relations between the reactions to be more apparent. They opt for 144 neurons arranged in a 12 by 12 grid. The architecture of the grid is therefore 12 x 12 x 6.

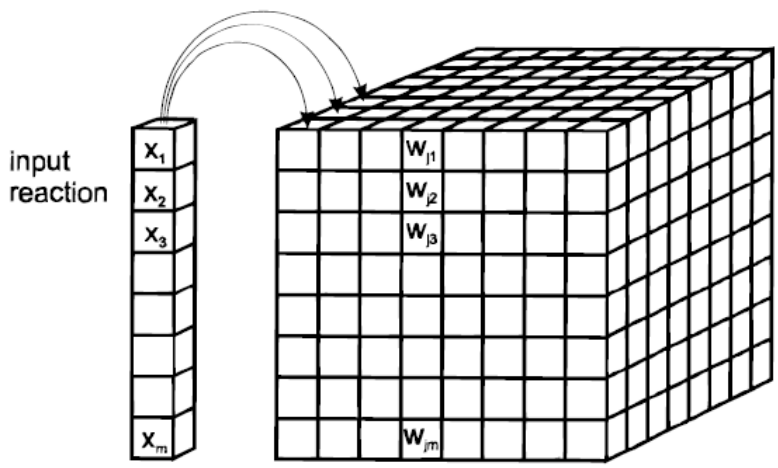


*Figure 3: Architecture of a neural network. Input vector X consists of m elements. Each neuron of the network is represented by a column with m weights (Gasteiger and Chen, 1997, 4034).*

The advantage of Kohonen network is that it is self-learning and doesn't require the target output of the system to be specified beforehand; the network adapts according to the original input values and so describes the original objects of investigation.

The training of the network begins by the initialisation of the neurons, in which the weights had by each neuron are assigned random numerical values. The next step is to feed an input vector into the network and identify the neuron which has weights most similar to the numerical values of the input vector. This is done by calculating the Euclidean distance between the input data vector xs and the weight vectors wj for all neurons. The neuron for which this distance is the smallest is called the winning neuron and is assigned that vector (i.e. that reaction). The process of calculating the Euclidean distances between reactions is achieved using the equation;

$\{\sum (xui - wji)^2 \rightarrow out_c\}$

The weights of the winning neuron are further adapted to the input data and the neurons within a certain distance surrounding the winning neuron are also adapted. The weight adaptation is performed so that the closer a neuron is to a winning neuron then the more its weights will be adapted.

The result of the neural network is a two dimensional representation of the reaction landscape. Each reaction is assigned a neuron, and in the case of very similar reactions, a neuron is occupied by more than one reaction. The respective positions of the neurons in the network (or reactions in the reaction landscape) represent the similarity relations that hold between the different reactions. The resulting visual representation of the reaction landscape allows complex data to be easily conceptualized and the similarity relations to be easily deciphered.

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 31 | 34 | 32<br>36 | | 41 | 42 | | 73 | | 54 72<br>60 | | 55 |
| 2 | | | 35 | | | | | 74 | | | | 53 |
| 3 | 2<br>3 | | 19 | | 43 | 40 | | | 67 | | 61 | 50<br>51 |
| 4 | | | | | | | 38<br>39 | | 62 | | | 52 |
| 5 | 1 | | 20 | | 49 | | | | | | | 57 |
| 6 | | | | | | 48 | | 45<br>46 | | 44<br>47 | | 56 |
| 7 | 12 | | 4<br>5 | | | | | | | | | 63 |
| 8 | 21 | | | 23 | | | | 27 | 28 | | | 59 |
| 9 | | 6 | | 22 | 10 | | | | | 30 | | 65<br>66 |
| 10 | 33 | 26 | | | | 15<br>16 | 17 | 18 | | | | 58<br>68 |
| 11 | | | 29 | 8 | | | 9 | | 11 | | | |
| 12 | 37 | | | 7 | 13 | 14 | | 25 | 24 | | 64 | 69 71<br>70 |

*Figure 4 Kohonen map obtained for the classification of 74 reactions (Gasteiger and Chen, 1997, 4036)*

For instance, the two dimensionality allows different types of similarities to be represented via neurons that exhibit a closeness in different directions on the landscape (up/down/left/right). The reaction landscape also reveals degrees of similarity; those reactions that are very similar appear very close together, those that are less similar are found further apart (Gasteiger, 2005, 192 - 196).

Finally a cluster analysis is performed to identify types of reactions as well as the similarities that hold between the individual reactions. This is again achieved by calculating the weight distances between neighbouring neurons using the Euclidean equation. This is represented in the diagram below via the height of the walls designating the different clusters.

The 74 different reactions are then interlectually assigned to groups according to theoretical knowledge to allow a comparison to be made. In both the reaction landscape and the theoretical groupings it was found that three general reaction types were present. These can be seen on the right hand side, centre and on the left hand side of the diagrams below.

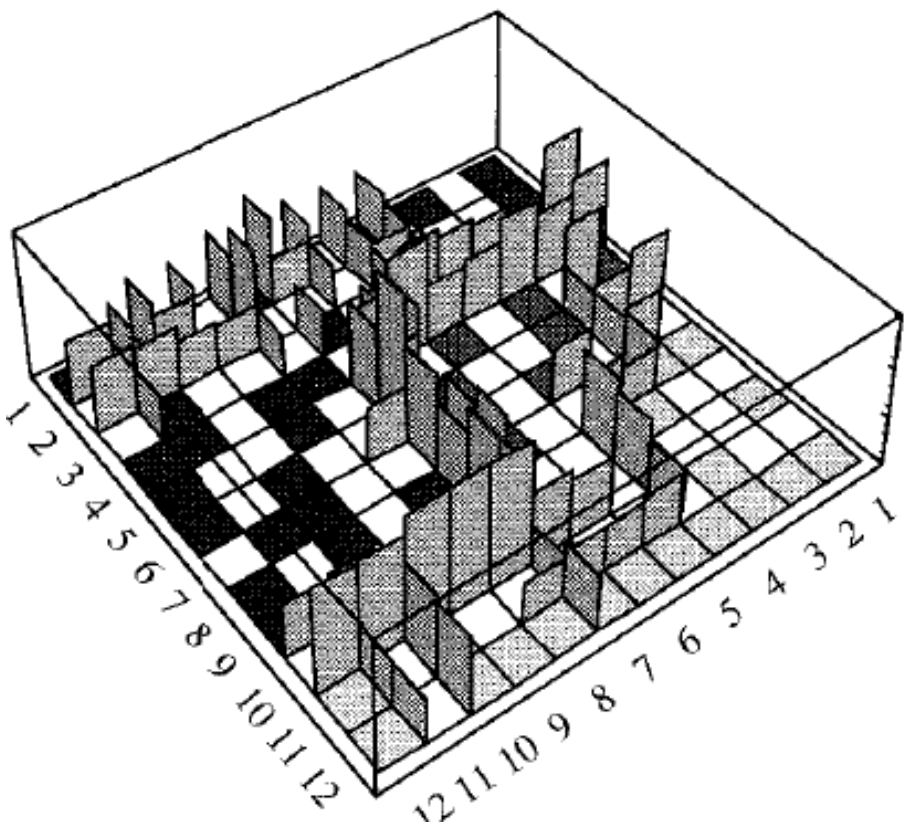


*Figure 5:Kohonen map for 74 reactions showing information on clusters detected using weight distance information. The wall indicated where the weight distance between adjacent neurons is larger than 0.85 (Gasteiger, 1997, 4039).*

A two dimensional representation is then produced in which the differnet cluster are represented in a different grey-scale.

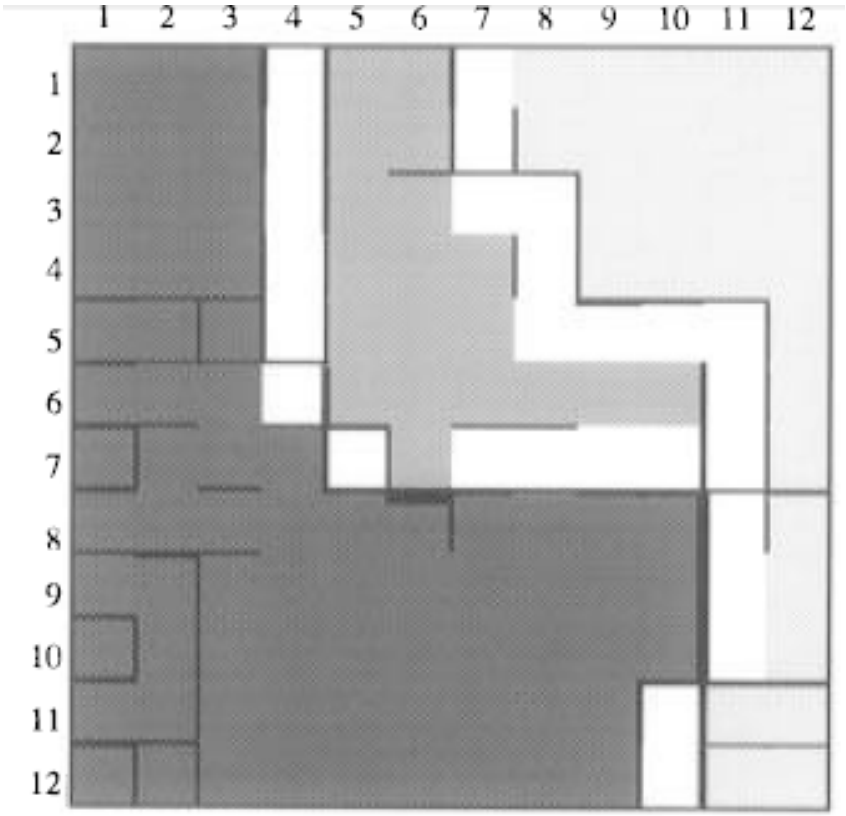


*Figure 6: Indication of the weight distance between adjacent neurons by the thickness of lines separating them. The occupied neurons are marked in different grey levels: dark grey indicates nucleophilic aliphatic substitution of acyl chlorides, medium grey stands for acylation of CdC bonds, and light grey stands for acylation of arenes (Gasteiger, 1997, 4036).*

In the reaction landscape resulting from the classification of the 74 organics reactions the dark gray colouring indicates the nucleopholic apliphatic sybstitution of acyl chlorides, the medium gray stands for the acylation of C=C bonds and the light gray stands for acylation of arenes. The intellectual classification was found to 'corrrespond quite nicely' to the automatic classification and it was concluded that using the weight - distance technique was an effective method for the automatic classification of reactions into 'chemically significant types‘ (Gasteiger, 1997, 4036).

The application of QSAR and neural networking to the classification of the initial 74 reactions successfully established that the procedure can obtain accurate results. The second part of this initial case study applies the procedure to a further

120 reactions in order to establish the amount of information that can be retrieved from the classification methodology. This second set of 120 reactions each involved an addition of an H-C bond to a C=C bond to form a C-C bond.

The reaction data was taken from the 1992 ChemInform RX database and the reactions were classified according to the following physicochemical variables;

1. Total charge

2. Sigma electronegativity

3. Pi electronegativity

4. Effective atom polarizability

These are the same properties as in the previous study however this time they did not take into account the values of the variables on all atoms of the reaction site instead they selected which properties of which atoms were most likely to be significant. The reason for this is that they wanted to show that a small set of variables deemed to be chemically significant can do the job of chemical classification.

> 'Rather than considering these four electronic properties on all atoms the full set of variables on all atoms of the reaction site can be used, or a subset of variables can be automatically selected by statistical methods. However, we have intentionally chosen the variables on the basis of chemical intuition in order to show how a small set of variables deemed chemically significant can do the job of reaction classification' (Gasteiger, 1997, 4038).

Figure 7 shows which properties were calculated for which atom. This was decided using theoretical insight from QSAR.

| | C | = | C | + | H | - | C | -> | H | - | C | - | C | - | C |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Total charge | | | x | | | | x | | | | | | | | |
| Sigma electronegativity | x | | | | | | x | | | | | | | | |
| Pi electronegativity | x | | | | | | x | | | | | | | | |
| Effective atom polarizability | | | | | | | x | | | | | | | | |

*Figure 7 Table showing the properties of the reaction centre that are relevant to classification (Gasteiger, 1997, 4038).*

This data was transported into a neural network following the process described previously and with the same sized grid of 12 x 12 neurons. This follows the general rule that the number of neurons should be between 1 and 3 times the number of reactions undergoing classification.

Once cluster analysis had been applied ten different reaction type clusters were correctly identified as corresponding to the standard classification model. These are shaded on the reaction landscape below. Among the reaction types identified were reactions of high importance in chemical synthesis including Michael additions and Fridel - Crafts alkylations in addition to more uncommon reactions like the hydride abstraction reaction. The resulting reaction landscape is shown below:

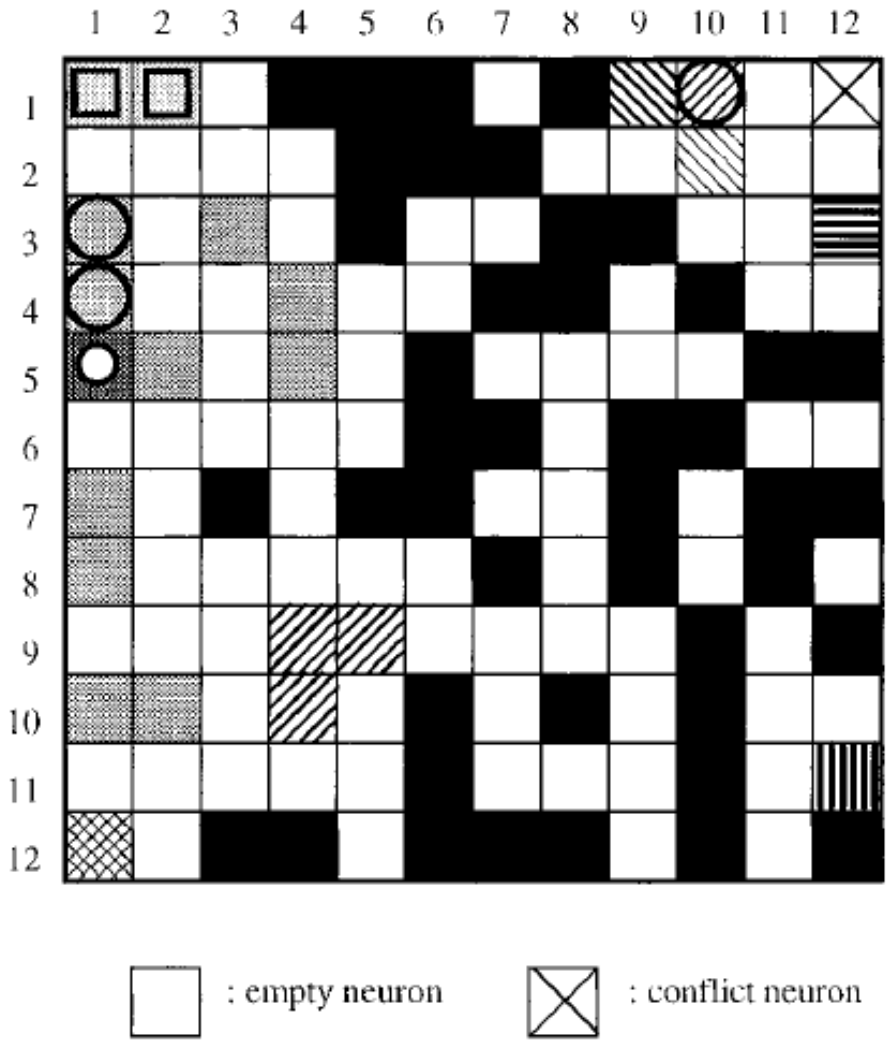


*Figure 8: Kohonen map obtained for the classification of 120 reactions that correspond to the key shown in figure 9 (Gasteiger, 1997, 4039).*

| | reaction type | number of reactions | index of reaction |
|---|---|---|---|
| A. | Michael addition | 75 | 1-14,24-84 |
| B. | wrongly assigned reaction center | 1 | 85 |
| C. | Friedel-Crafts alkylation by alkene | 18 | 15-23, 86-92, 115, 116 |
| D. | electron transfer reaction | 1 | 93 |
| E. | photochemical addition of acyl radical to electron-deficient alkene | 1 | 94 |
| F. | photoinduced alkylation reaction | 4 | 95-97,101 |
| G. | hydrogen atom (radical) transfer reaction | 3 | 98-100 |
| H. | reaction with special reaction mechanism | 1 | 102 |
| I. | hydride abstraction reaction | 3 | 103-105 |
| J. | Nazarov reaction | 5 | 106-110 |
| K. | allylation of a keto ester followed by anti-Markovnikov addition of HBr (2-step-reaction) | 1 | 111 |
| L. | palladium-catalyzed oxyhexatriene cyclization (2-step reactions) | 3 | 112-114 |
| M. | condensation reaction | 1 | 117 |
| N. | photoinitiated radical addition of a crown ether | 3 | 118-120 |

*Figure 9: Intellectually assigned reaction types, associated symbols, and the corresponding number of reaction instances in the classification of 120 reactions as shown in Figure 8, (Gasteiger, 1997, 4039).*

The large amount of chemical information that is stored within a reaction landscape can be demonstrated through an analysis of the Michael addition reaction

type as identified in figure 7 and 8. These 75 reactions were mapped into 43 neurons which is indicative of the chemical variety within the group. Further sub-clusters can be identified within the Michael addition group that correspond to types of electron withdrawing group and the number of electron withdrawing groups; figure 9 represents variation of electron withdrawing groups within the cluster. The neural network also reveals special cases of Michael additions; these are found at the borders of the cluster as demonstrated by figure 10 (Gasteiger, 1998, 218).

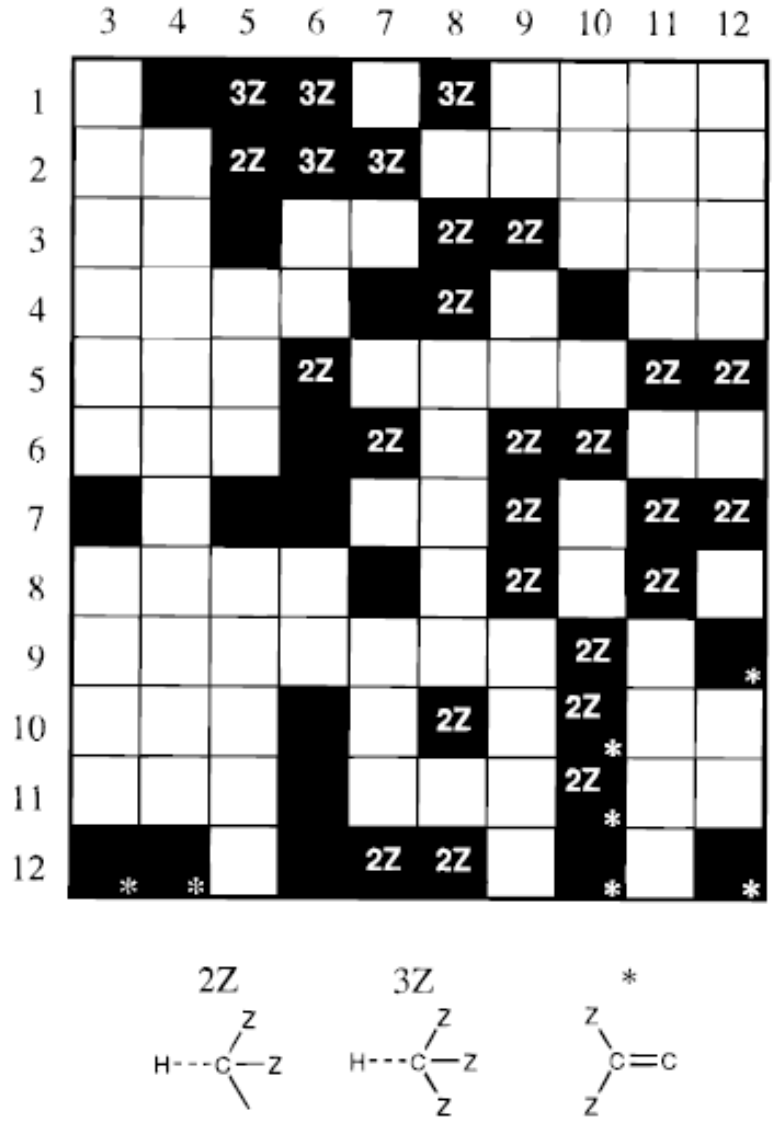


*Figure 10: A representation of Michael addition reactions where z corresponds to the number of electron withdrawing group in each Michael addition. 2Z = Two electron with drawing groups at H-C. 3Z= three electron with drawing groups at H-C *= Two electron withdrawing groups at C=C (Gasteiger, 2007, 4040).*

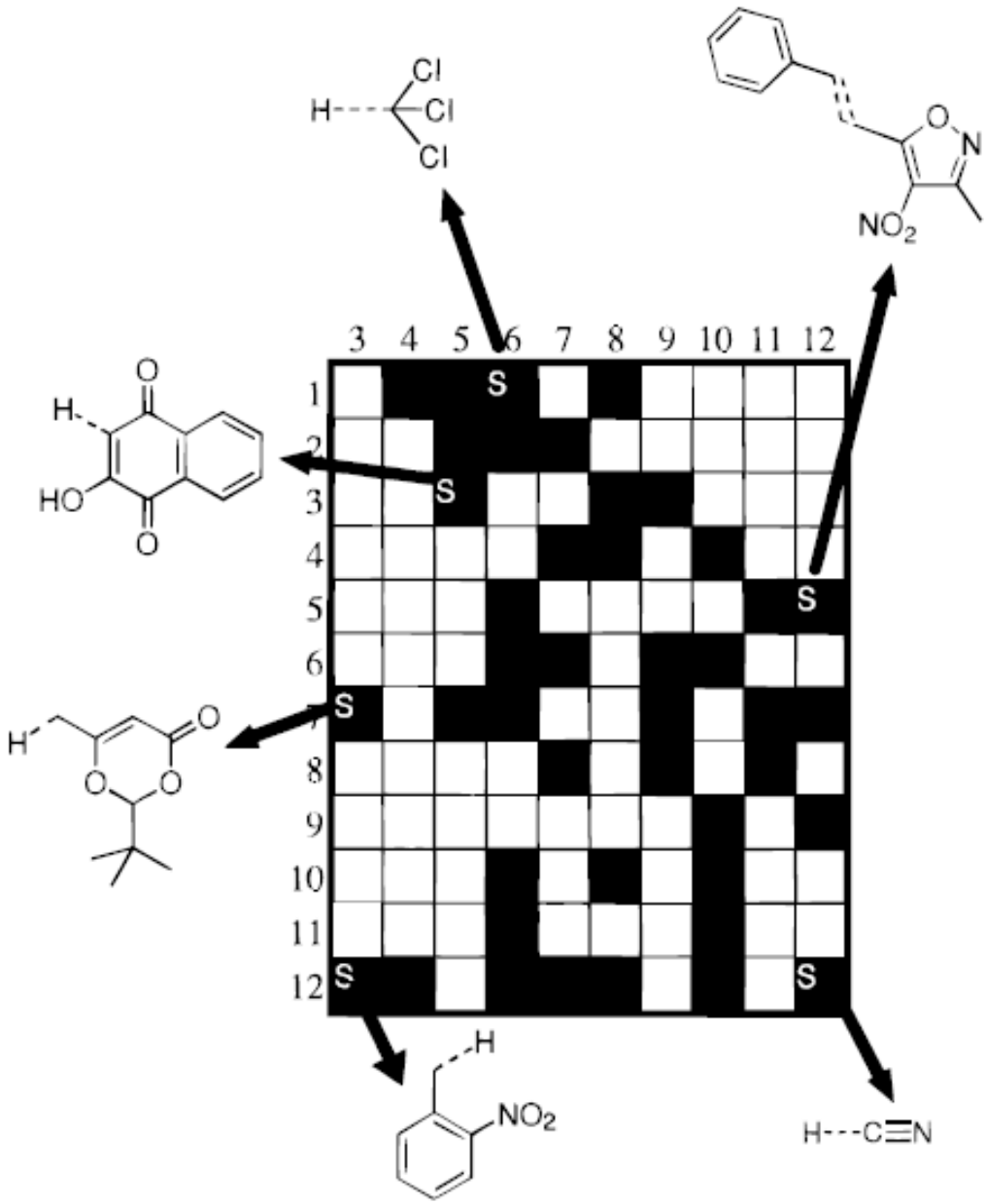


*Figure 11: representation of special cases of Michael addition reactions (S) found at the boundaries of the cluster (Gasteiger, 2007, 4040).*

It is interesting to note that in the method just described no attention is paid to the functional groups at the reaction centre and in the immediate reaction environment. This approach can be compared to another method of classification developed by Gasteiger and Rose; the Hierarchical Organization of Reactions though

Attribute and Condition Education, also known as HORACE (Rose and Gasteiger, 1994).

HORACE had a multi-tier approach to classification in which reactions were classified according to physicochemical variables as above and then according to functional groups with this process repeating until only the individual reactions remained. Initially reactions were classified on the basis of their physicochemical features such as charge distribution as well as inductive and resonance effects at the reaction centre. The classes of reactions that were identified were then further sub-classified according to topological features such as the presence of simple functional groups (alcohol, carbonyl etc.). The resultant groups were then fed back into the system and further sub sub classified on the basis of physicochemical and then topological features.

When the HORACE system of classification was applied to the same set of reactions from the ChemInform RX database described in the previous case study, it was found to perform less well than a classification just on the basis of physicochemical variables. The Horace system grouped the reactions into a larger number of reaction classes and so was not able to recognise more coarse grained similarities between the kinds. It was constrained by the need to accommodate topological similarities. In other words to recognise similarities in the structural arrangement of molecules as well as similarities in the physicochemical variables associated with reaction centres. This problem can be most clearly demonstrated by the treatment of the Michael addition reactions. Horace would have classified these into 20 distinct reaction classes whereas chemical intuition and the methodology described above would have identified them as falling into one group. The advantage of the neural network approach to classification is that it is able to recognise both coarse and fine grained similarities, grouping reactions into fewer classes but also representing lower level variation by identifying the locations of reactions within the cluster (Gasteiger, 2005, 191).

## 2:3: Initial Requirements on a Metaphysics of Classification

The aim of the previous section was to outline an approach to the classification of chemical reactions focusing on the use of QSAR and neural networking to produce a representation of the similarity relations that hold between reactions. In this section, I will use this discussion to draw out initial constraints on a metaphysics for the classification of reactions concerning, the three stage classification process, activities as heuristics and the role of representation. Any metaphysical account of classification must be compatible with these criteria if it is to accommodate the classification of chemical reactions in practice.

### 2.3.1: Three stage classification

The classification of chemical reactions takes place in three stages. Firstly, a rough classification is used to identify a set of reactions that on the basis of prior theoretical knowledge are known to be similar to each other. Typically, this involves identifying reactions with similar reaction centres. The term ‘reaction centre' refers to parts of the molecules that are involved in the making and breaking of bonds during the reaction. I refer to the identification of reactions with similar reaction centres as the first stage of classification. The motivation for this step is that reactions involving the same atoms and bonds must share some basic higher level similarities. The second stage of classification is the application of QSAR and the third stage of classification is the application of neural networking which provides a more refined classification of this set of reactions. This whole process identifies more fine grained similarities between the reactions that are initially identified as similar.

The first stage of classification is a crucial component of the classification process since it enables the successful application of QSAR. The QSAR relation should apply to all reactions under investigation, in virtue of all reactions being the same type of activity. If the reactions are already similar then a more in depth QSAR analysis can be provided. In the case studies described above it was already established that all the 120 reactions were all organic reactions involving carbon and

oxygen, this meant that chemists could appeal to their own theoretical knowledge to isolate the factors that determine how the reaction centres of that kind are likely to change under different conditions.

If the reactions under investigation are not closely related then the application of QSAR will be less effective for it will be different underlying structural properties that are responsible for the instantiation of the different reactions. In this sense the activity referred to in QSAR acts as a heuristic device, guiding the second stage of classification. The properties that encode the reaction and on which the classification is based are chosen because they best describe that activity of interest (i.e. the reaction), if chemists were interested in a different activity then different properties would be used. A metaphysics of classification must be able to accommodate this multi stage classification process, this means a successful metaphysics must be compatible with other methods of classification that provide a more general grouping that can be then further refined.

### 2.3.2: Unification and Activities as Heuristics

In chapter 1 I discussed a debate specific to classification in chemistry concerning the types of properties we should use for classification. On the one hand Hendry's microstructuralism maintains that classification should take place at the level of micro properties, whilst Needham and van Brakel argue that classification must take place at the macro level in order to accommodate thermodynamic properties of substances.

I outlined this debate in the context of how to specify the identity conditions of water and described the standoff that results. Microstructuralism defines the extension of the term 'water' in terms of the substance's microstructural properties. The view trades on the modal intuition that if two substances have the same manifest properties but different microstructures we would consider them to be different substances. Hendry accepts that more complex substances such as water are macroscopic substances with thermodynamic properties but does not take these

properties to be relevant to classification. Melting point, boiling point, thirst quenching ability etc. are all used to identify water but these properties do not make substances such as water what they are. Instead, Hendry asserts that water is produced by bringing together $H_2O$ molecules so on his view it is $H_2O$ molecules that determine the extension of the term.

Needham rejects this thought experiment on the grounds of its implausibility; current scientific knowledge indicates that it is not possible for two substances to be indistinguishable at the macro level and different at the micro level and so the modal argument for microstructuralism bears no weight. Needham is driven by the intuition that the properties on which the classification are based should play an explanatory role. For example complex substances such as water cannot be given microstructural definitions such as 'water = $H_2O$' because a single $H_2O$ molecule will not have the manifest properties associated with water. Rather melting, boiling and thirst quenching are all properties that are explained by the complex interaction between $H_2O$ molecules and its environment. In addition, the structure of this interaction depends on the state water is in; water in the form of liquid has a very different microstructure to water in the form of gas or ice. Therefore whilst 'water = $H_2O$' is an incomplete microstructural account, it is unclear whether a more specific characterisation that applies to ice, liquid water and steam can be given.

In chapter 1 I also described Needham's claim that for complex substances thermodynamics should be used to determine the extensions of kind terms. I concluded in chapter 1 that we are left with a standoff between microstructuralists who are persuaded by the modal argument that microstructural properties have priority when classifying and their macro opponents who argue that thermodynamic properties have explanatory priority and that this is more important in classification. Having analysed the way in which classification takes place in practice I argue that the first part of the classification methodology has important implications for the microstructural classification versus thermodynamic classification debate in the philosophy of chemistry.

In an ideal world chemical reactions would be classified according to similarities in their individual reaction mechanisms, however as I explained at the start of this chapter this information about reaction mechanisms is beyond the scope of current science. Instead reactions are classified according to physicochemical variables which are thought to be the best possible indicators of what these reactions mechanisms would be like. The application of QSAR stems from the belief that similarities in structural properties result in a similarity in higher level phenomena. This means that in practice chemists treat a difference in macro level or thermodynamic properties such as an instance of a chemical reaction as indicative of a difference in the lower level properties underlying that reaction. The idea is that once the relevant structural properties have been identified they can be used to better classify the macro level activities or in this case reactions.

This claim might be thought to favour microstructuralism and the notion that it is structural properties that are central to classifying higher level types. However I suggest that classification using QSAR is more complicated. Rather than automatically seeking to classification on the basis of structural properties, the aim of QSAR is instead to provide a unification of microstructural and higher level (macro, manifest or observable) properties. The classification must take place at the level that best reveals the similarities that hold between the phenomena of interest. In some cases this will involve a classification in terms of the microstructural arrangement of atoms and bonds but sometimes the structural properties referred to by QSAR will be at the thermodynamic higher level. In all cases the level at which the classificatory properties are found should be the level that best captures the similarities that the chemist is interested in. Rather than prefer micro or macro approaches to classification as advocated by Hendry or Needham we should look at which properties best capture and explain these similarities.

We can also conclude that higher level or manifest phenomena are always relevant to the classificatory process in the sense that they provide a heuristic device for identifying lower level variation. The job of scientists is to identify the level at which we find the properties responsible for these higher level differences. In the

case of chemical reactions it is physicochemical variables that best describe the behaviour of reactions but in the case of water perhaps a thermodynamic specification would be most appropriate when employing QSAR. If we wanted to predict the manifest properties of water then a structural account of the arrangement of $H_2O$ molecules in long chains that continually disassociate and then re-associate would be most appropriate. It is this process that is responsible for the observable properties of liquid water.

## 2.3.3: Role of Representation

In addition a metaphysics of classification must be compatible with the role of representation in chemical practice. Assigning a role to representation in classificatory procedures is common place when considering the classification of entities. For example, when classifying chemical entities it is the representation of individual entities that is important; consider the case of microstructuralism as discussed in chapter 1. The microstructuralist individuates chemical entities solely in terms of their chemical microstructure. I described how this approach is sufficient for elements that are individuated in terms of their atomic number but for more complex molecules an additional appeal to molecular arrangement is also required. Therefore the representation of the molecular structure, including features such as bond angles and bond length are also required.

Providing a structural representation of entities allows chemists to distinguish between isomers that contain the same constituent parts in different arrangements thus forming chemically distinct molecules with different behavioural properties. In addition, in the case of more complex molecules features such as bond angles and charge are continuous variables and this leads to vague boundaries between different kinds.

My case study sees the role of representation in classification expanded by representing not the individual entities or reactions, themselves but the relations that hold between all the distinct reactions undergoing classification in the neural

network. I suggest this has at implications for how we think about the philosophy of classification, and introduce the notion of a the 2-dimentionality of the classification scheme.

Typically chemical classification proceeds by the identification of a type and then the accumulation of a list of tokens that instantiate that type. I call the classification of tokens into types a 1-*dimensional classification scheme*. It is 1-dimensional because the output of the classification amounts to a list of instantiations of that kind. Consider the classification of acids, all acids have in common the property molecule or other species which can donate a proton or accept an electron pair in reactions. We know that examples of acids include Perchloric acid, Chloric acid, Chlorous acid, Hypochlorous acid and Hydrochloric acid, however no further details can straightforwardly be given on how the different tokens listed as a member of the kind relate to one another. What similarities hold between the token instances that constitute members of that kind? A 1- dimensional classification scheme is unable to answer these questions.

The representation of reactions in the case study described above is, in contrast a 2-dimensional classification scheme. Whilst this reaction landscape is divided into clusters corresponding to preassigned types, on a 2- dimensional account the information conveyed on the reaction landscape is not reduced to types and a list of corresponding tokens. Instead the chemist is able to assess the broader classificatory picture by analysing the representation, in particular;

a. The degrees of similarity that hold between any two token reactions. For example consider the bottom row of the reaction landscape in figure 3. Reaction 7 is more similar to reaction 13 than reaction 12 because reaction 7 is closer to reaction 13.
b. The types of similarity that hold between any two token reactions. For example, consider the top row of the reaction landscape in figure 3. Reaction 73 is similar to reaction 42 but is also equally similar to reaction 54, though this similarity is in a different respect. This is illustrated by a closeness in different directions on the reaction landscape.

c. The relative similarity of one type of reaction to other types appearing on the reaction landscape.

In so far as the aim of classification in chemistry is to further scientific knowledge by making accurate predictions then a 2-dimensional classification scheme is an advantage. A better understanding of the similarity relations that hold between reactions paves the way for better predictions. A 1 - dimensional scheme fails in this regard due to a lack of information content. In some cases, in a 1-dimensional reaction scheme the option is available to divide the members of a type into subtypes and produce a hierarchy of kinds however it is still not clear how the different subtypes relate to one another or indeed relate to the overall type. Additionally we have no further information on how members of each subtype are similar to each other than in virtue of sharing a common property. A 1- dimensional classificatory scheme amounts to a list of qualifying entities. This is helpful for organising scientific knowledge but it is not as useful for making predictions.

To conclude this section, I have so far outlined a methodology for the classification of chemical reactions used in practice and shown the results of its pioneering application to the classification of organic reactions. From this I have drawn a number of implications for a metaphysics for the classification of chemical reactions. Such a metaphysics must be compatible with a multistage classificatory procedure in which chemists appeal to rough classifications of reactions in order to identify those reactions that could fruitfully be classified further using QSAR and neural networking.

I also showed that the application of QSAR has implications for the debate between microstructuralists and their macro opponents. The aim of chemists is to provide a unified account of lower level structural properties and a higher level activity such as a particular sort of reaction. In this sense activities have a vital role in acting as heuristic devices. A difference in a higher level activity is thought to be indicative of a difference in the lower level structural properties responsible for producing that activity. In addition, whilst chemists speak of structural properties, it is not the structural arrangement itself that is used to classify reactions as

microstructuralism asserts, but rather the physicochemical properties that are indicative of structure. The resulting classifications are used to make predictions and are therefore thought to latch on to real reactions in nature.

I also showed the importance of representations of 2-dimensional classificatory schemes and suggested that it is the 2-dimensional representation that has predictive priority as it is able to reveal degrees and types of similarities in each case.

## 2:4: Recent Applications: the Classification of Enzymatic Reactions

The previous case study involved the classification of organic reactions primarily in order to test the classification procedure. However, the following more recent case study shows how the same methodology can be used to produce a more refined classification of reactions in order to achieve an certain practical end.

The aim of the investigation is to use QSAR and neural networking to classify enzymatic reactions, producing for enhanced predictive ability and the fruitful development of science. The output of the classification scheme is the identification of similarity relations between the enzymatic reactions undergoing classification and the grouping of similar reactions together into clusters. This is important in light of the additional assumption that similar reactions will react in the same way to changes in environmental conditions such as temperature, pressure and substrate concentration. The resulting chemical knowledge is then fed back into chemical theory allowing for greater explanatory unification. Improved knowledge about the similarity relations between reactions allows chemists to build up a picture of why these reactions have certain optimum conditions and the ways these can be manipulated. This in turn leads to greater predictability.

This case study has an additional element since a better classification of enzymatic reactions allows for a refined classification of enzymes themselves.

Enzymes are proteins and they are classified into types and sub-types using the EC system of classification. Each unique enzyme is identified using four digits in the form a.b.c.d. The first number, a, gives the main class to which the enzyme belongs of which there are six options, 1. transferases 2. hydrolases 3. lyases 4. isomerases 5. ligases 6. oxidoreductases. Each class is then further divided into subclasses (b) which are then subdivided twice more (c,d) (Sacher, Reitz, Gasteiger, 2009, 1525).

The classification system is designed so that enzymes are classified according to their functional ability to catalyse reactions, therefore a classification of enzymes, is dependent on a classification of enzymatic reactions. A more refined classification of enzymatic reactions will in turn lead to a more refined classification of enzymes. The motivation is that the application of the classification procedure would reveal unknown similarities between enzymes and thus reveal new uses for existing enzymes.

The investigation is described in a 2009 paper entitled *Investigations of Enzymes Catalyzed Reactions based on Physicochemical Descriptors applied to Hydrolases.* It involved a data set taken from the Biopath database (Sacher, Reitz, Gasteiger, 2009). Before discussing the classification procedure and output it is useful to understand where the data on which the classification is based originates from.

## 2:4:1: Creation of the Biopath Database

Over the past four decades huge amounts of information have been collected concerning the chemicals that exist within each animal cell and the ways in which these chemicals interact with each other. This information was collected and assembled by G Michal and displayed in the Biopath wall chart in 1965. This went on to become a staple reference resource found in biochemical laboratories around the world. Its success is due to its ability to represent large amounts of data.

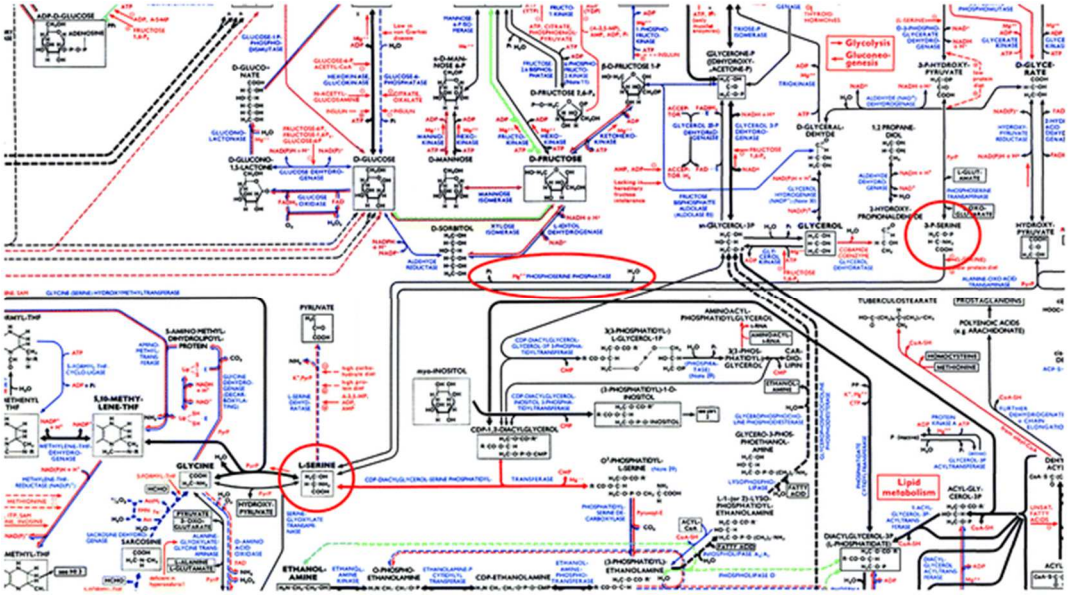


*Figure 12: the Biopath Wall chart (Reitz, Sacher, Tarkhov, Trumbach, and Gasteiger, 2004, 3226)*

The Biopath wall chart has the disadvantage that information retrieval is difficult, particularly if chemicals are located at more than one place on the map. 'Relationships between many compounds through a large number of relations have to be stored in a two-dimensional place. This can only be achieved by large distortions and an awkward arrangement of reaction arrows, ostensibly for reasons of clarity' (Reitz & Sacher, 2004, 2226)

In 2004 a project to transfer the information contained within the Biopath wall chart to a database was completed to better meet the practical needs of chemists. All information contained within the Biopath database is obtained empirically. Chemical structures are represented by connection tables which contain lists of all atoms and all bonds involved in each reaction. Chemical reactions are specified by the start and end products of a reaction as well as the enzymes involved. All bonds broken and made in the reaction are identified with every atom found in the starting materials and those atoms found in the products mapped against each other. All reaction equations are balanced with the involvement of protons in the starting materials specified in the reaction equation to ensure accuracy.

In addition, for each reaction, information is given on whether it is a general pathway or whether it occurs in animals, plants, yeasts etc. The location of where the

reaction typically occurs is specified alongside details concerning whether it is a reversible or irreversible or catabolic or anabolic reaction.

## 2:4:2: Application of QSAR and Neural Networking to Enzymatic Reactions

The classification of hydrolysis enzymatic reactions (and the resulting classification of hydrolase enzymes) was produced using a combination of QSAR and neural networking. The project began by isolating the structural properties of the reaction centres of the constituent entities that best indicate the type of reaction that will be instantiated in each case. These properties ensure all major electronic effects of reaction mechanisms such as charge distribution, inductive, resonance and polarizability effects are taken into account. Each reacting bond is assigned a value for each property with this data imported from the Biopath database.

As in the previous case study, each reacting bond is characterized by six properties however in some of the reactions two bonds were broken and therefore each reaction was encoded by a vector of length twelve. Those reactions that only broke one bond were assigned a value of zero for the gaps in the vector. This twelve dimensional space was then projected into a two dimensional space using a neural network following the process described in section 2.2. These properties are similar to those identified in the previous case study:

1. Difference in partial atomic charges which describes the polarity of the bond
2. Difference in sigma electronegativities which describes the ability of an atom to attract electrons in a sigma bond[9]
3. Difference in pi electronegativities which describes the ability of an atom to attract electrons in a pi bond [10]

[9] A Sigma bond is the strongest type of covalent bond formed by a head on overlapping of atomic orbitals

[10] A Pi bond is a weaker form of covalent bind due to a reduced overlapping between the atomic orbitals

4. Effective bond polarizability which describes the tendency of the bond electrons to be distorted by an external electrical field
5. Delocalization stabilization of a negative charge on reaction centre which describes the stabilization of a negative charge generated by the heterolysis of the bond[11]
6. Delocalization stabilization of a positive charge on reaction centre which describes the stabilization of a positive charge generated by the heterolysis of the bond

Clusters of similar enzyme catalysed reactions were identified on the basis of the Euclidean distances of the weight values of the adjacent neuron pairs. Neighbouring neurons that show small weight distances are quite similar and may belong to the same cluster whilst large weight distances between neurons are indicative of separate clusters of reactions.

Once the reaction landscape had been produced the neurons representing each reaction were then matched with the enzyme responsible for catalysing them and they were coloured appropriately. Neurons which contain reactions that correspond to more than one EC class were identified as conflicting neurons and were given multiple colours (Sacher, Reitz, Gasteiger, 2009, 1529).

The investigation began by producing an overall classification of all reactions involving enzymes in the category EC.3.b.c.d. Then in those cases where enough token instances of reactions were available then individual subclasses were analysed, these were subclasses EC 3.1.c.d, EC. 3.2.c.d and EC 3.5.c.d.

[11] A heterolysis bond is one in which the process of breaking a covalent bind in which the shared electrons are claimed by one of the chemical species.

*EC 3.b.c.d*

In the classification of the class EC 3.b.c.d all 135 reactions involving hydrolase were assessed. The resulting reaction landscape shown in figure 13 shows a clear separation of reactions into two groups which are indicated by a dashed line. On the right hand side of the landscape is a cluster of reactions belonging to subclasses EC 3.5.c.d and 3.1.c.d. All of these reactions have in common that they break two bonds during the reaction. On the other side of the dashed line are reactions in which one bond is broken. In addition, it is noted that the reaction landscape reveals clusters where all members undergo a change in bond order, with cases in which a double bond is converted into a single bond are indicated. It is stated that 'by and large, the similarity analysis of reactions based on physicochemical descriptors reproduces the classification of enzymes by the EC number' (Sacher, Reitz, Gasteiger, 2009, 1529).

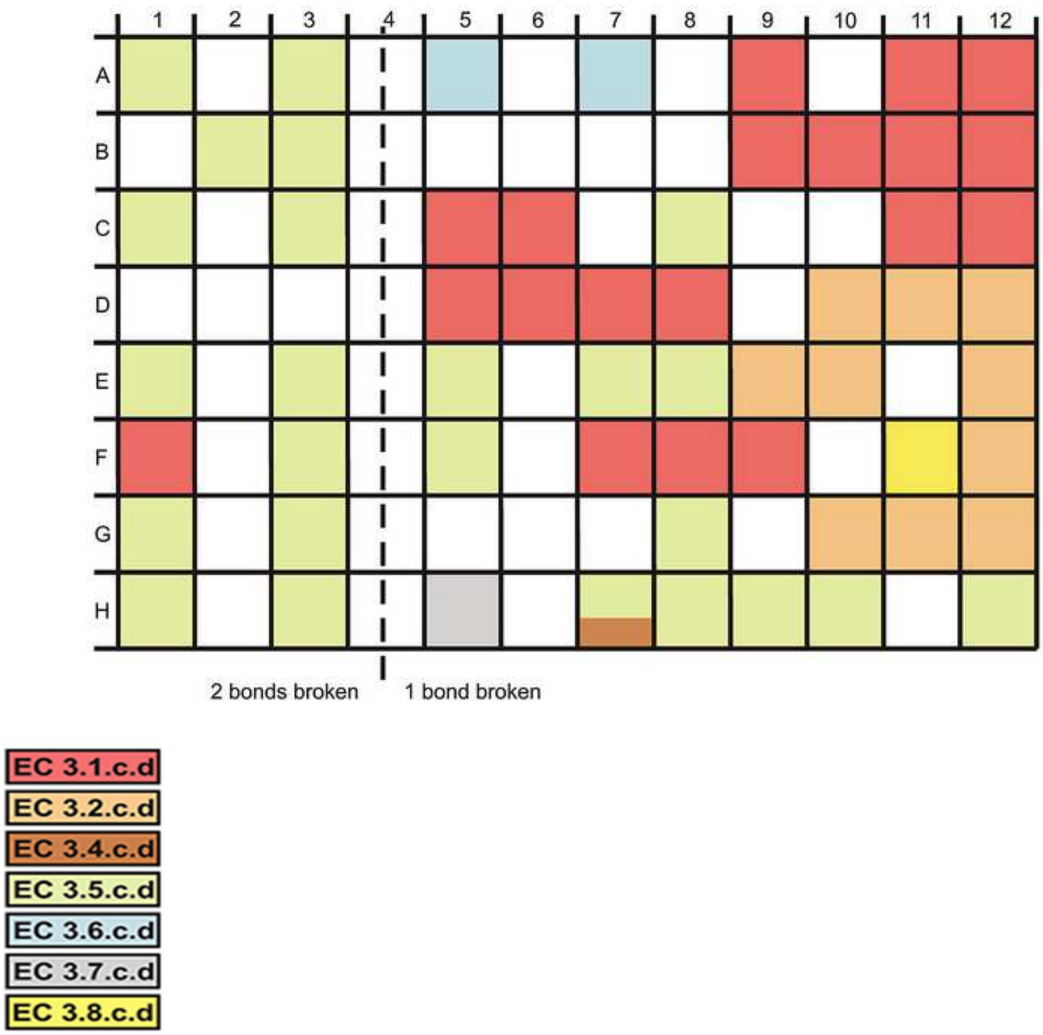


*Figure 13: Projection of reactions in class EC 3.b.c.d into a neural network (Sacher, Reitz and Gasteiger, 2009, 1529)*

*EC 3.1.c.d.*

Secondly a classification is produced for the subclasses of hydrolase reactions beginning with the group EC 3.1.c.d. The resulting classification scheme can be seen below and is clearly divided into four clusters.

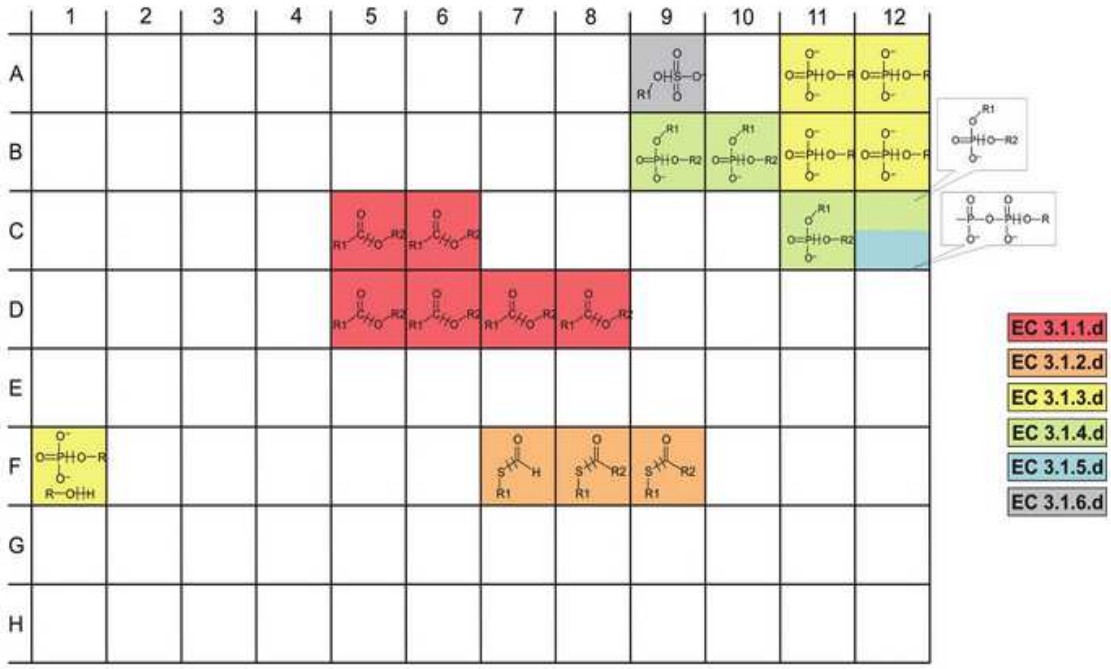


*Figure 14: Projection of reactions in class type EC 3.1.c.d in to a neural network (Sacher, Reitz and Gasteiger, 2009, 1531)*

The cluster in the centre of the landscape coloured red consists of the reactions catalysed by enzymes from the sub-subclass EC 3.1.1.d known as carboxylic ester hydrolases. The second area coloured orange contains reactions catalyzed by enzymes from EC 3.1.2.d known as thioester hydrolases. The third cluster in the top right hand corner consists of three subclasses of reactions; those enzymes classified as EC 3.1.3d marked in yellow, enzymes classified as EC 3.1.4.d marked in green and EC 3.1.6.d marked in grey. Finally, the fourth area is located on neuron F1 which contains only one reaction.

The classification was also able to reveal a coding error in the Biopath. The reaction catalysed by enzyme EC 3.1.3.36 appeared a long way from other reactions that are catalysed by members of the class EC 3.1.b.c. This is because the enzymes

originally catalysed as EC 3.1.3.36 in fact belonged to the group EC 2.7.1.137. Overall the classification of reactions of this subtype was deemed to be successful.

<u>EC 3.2.c.d</u>

Nineteen reactions of this subclass were classified resulting in a clear separation of the reactions into the two subclasses EC 3.2.1.d and EC 3.2.2.d. This was as expected and was without any conflicts. There is also a clear separation with the type of bonds broken. Reactions catalysed by enzymes from the EC 3.2.1.d class involve the breaking of the O -glycosidic bond; a type of covalent bond that joins a carbohydrate molecule to an oxygen. Reactions catalysed by enzymes from the EC 3.2.2.d group involve the breaking of an N- glycosidic bond which joins a carbohydrate molecule to a nitrogen atom.

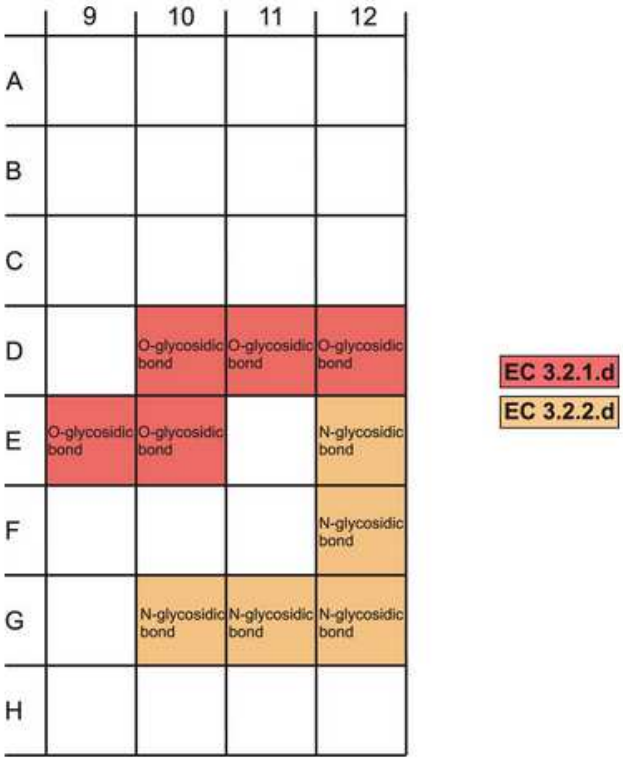


*Figure 15: the projection of reactions in the class EC 3.2.c.d into a neural network (Sacher, Reitz and Gasteiger, 2009, 1532)*

EC 3.5.c.d

In this final classification 44 reactions of subclass EC 3.5.c.d were classified using a neural network with the results shown in figure 16. The enzymes involved are known to involve hydrolase acting on a carbon- hydrogen bond. Firstly the classification shows a clear separation between those reactions where two bonds are broken and those where one bond is broken.

Reactions are also clustered according to the kind of molecules involved in the reactions, for instance, there is a clear separation between reactions that involve purines and reactions that involve pyrimidines. There is a further separation between those reactions that occur at different positions on the purine rings.

Finally, the classification reveals reactions that are clustered according to similarities in the substructures of reactions including reactions that involve the breaking of the primary aminde and release of ammonia, the hydrolysis of the primary amide and the hydrolysis of the formyl residue. The resulting classification confirmed the original EC classification scheme but also advanced our knowledge of enzymatic classification through the identification of new reactions within clusters that are linked to certain enzymes.

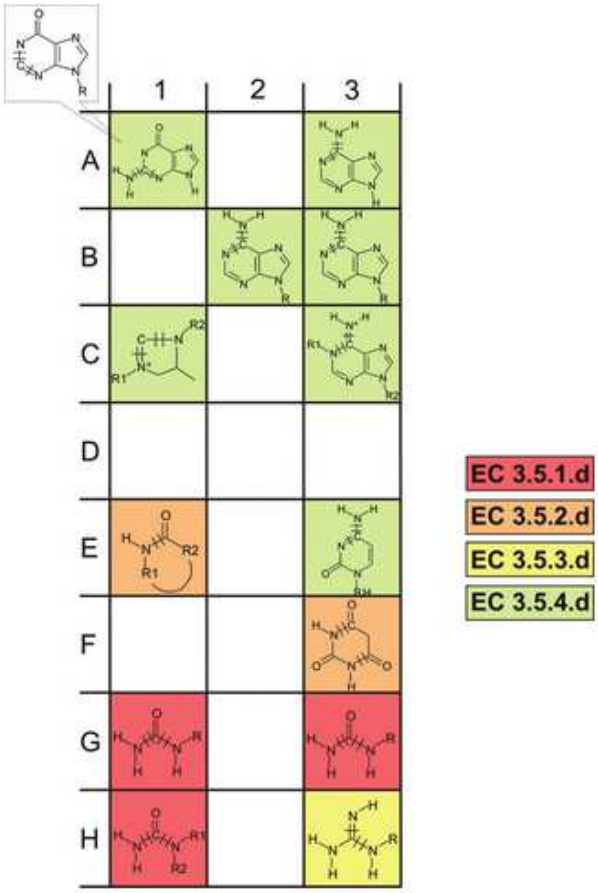


*Figure 16: projection of reactions from the class EC 3.5.c.d into a neural network (Sacher, Reitz and Gasteiger, 2009, 1532)*

The aim of the investigation has been to apply a classificatory procedure to a set of reactions that are known to be similar to each other. This allows a more refined classification of the types which reveals additional subtypes and ensures a greater level of predictability. Knowledge of the way in which one reaction behaves under certain environmental conditions can inform predictions about the way in which other reactions will behave under the same conditions. These predictions will be more accurate the more refined the classification scheme is. It is claimed that; 'this similarity analysis reveals finer details of the enzymatic reactions and thus can provide a better basis for the comparison of enzymes' (Sacher, Reitz, Gasteiger, 2009, 1534).

## 2:5: General Requirements on a Metaphysics of Classification

In section 3 of this chapter I outlined some initial requirements that a metaphysics of the classification of chemical reactions must be compatible with. This involved activities (or reactions) acting as heuristic devices, the three stage classification process and the role of representation in the production of the reaction landscape. Having outlined the classification of enzymatic reactions in section 4 I will now broaden this discussion and will argue that a metaphysics for the classification of reactions must also be descriptively fit for purpose. To be descriptively fit for purpose an account of classification must adhere to three general criteria; descriptive accuracy, capture similarity relations and promote explanatory unification.

The aim of my project is to provide a metaphysics for the classification of reactions as this occurs in everyday life of the chemists. This is a particular brand of naturalised metaphysics that I have termed *descriptively fit for purpose*. It is led by the aims and interests of scientific inquiry and should facilitate scientists meeting the end goal of their investigation. Nonetheless, I acknowledge that this approach to addressing metaphysical questions is controversial and that appropriate methodology within metaphysics is hotly contested. This is with regards to balancing ontological strength with the principle of parsimony as well as the relation between science and metaphysics (Quine, 1948, 1969) (Lewis, 1973) (Schaffer, 2004) (Ladyman and Ross, 2007) (L.A. Paul, 2012). I follow the approach of Illari and Williamson (2013) in making the requirements on a metaphysical framework explicit from the outset and analysing each metaphysical candidate with respect to these criteria.

### 2:5:1: Descriptive Accuracy

My project is to produce a metaphysics of classification of reactions in practice and in order to accommodate practice it is essential that such an account is descriptively accurate or rather descriptively accurate enough to meet the aims of the inquiry. I have in mind the sort of naturalized metaphysics advocated by Ladyman

and Ross in their *Everything Must Go.* They advocate the claim that certain types of contemporary analytic metaphysics fails to contribute towards the enlightened pursuit of knowledge, suggest that it has lost sight of its raison d'etre, employs a misguided methodology and should be discontinued. They argue that this is due to contemporary analytic metaphysics being preoccupied with domestication; the desire to render science compatible with our folk intuitions on issues such as structural composition and causation. More often than not domestication involves preserving what is referred to as the containment metaphor, the view that the world is structurally composed of tiny building blocks of matter, where causation is to be explained in terms of the collisions between such particles. It is argued that such domestication is destructive to the enterprise of metaphysics, since it is based on outdated and refuted scientific theories. Insofar as the aim of metaphysics is to provide an objective account of the structure of reality and the best source of evidence available to metaphysicians about the nature of this reality is provided by natural science, the best metaphysics will be one that takes into account natural science. Consequently metaphysics should not contain claims that are inconsistent with theoretical knowledge for example claims that are known to be empirically inaccurate.

It is worth noting however that the criterion of descriptive accuracy is always relative to the aims and interests of chemists. Earlier in this chapter I discussed how it is the chemists' interest in a particular activity that drives QSAR and determines the direction of their investigation. Chemists investigating two different phenomena may choose to ignore or abstract away from or focus in on different chemical details accordingly. Those descriptive inaccuracies that do not affect the classification process are permissible. To capture this point I will at times discuss whether an ontology is descriptively accurate *enough.* There is a further question whether the classifications themselves and the notion of descriptive accuracy at play are interest dependent such that they will change as interests change. I will address this point in chapter 6.

## 2:5:2: Identification of Similarity Relations

I previously described how the aim of the investigation in case study two is a growth in the knowledge of different enzymes and an understanding of how this scientific knowledge can be manipulated to produce greater predictive accuracy. The output of the classification schemes is the identification of similarity relations between the enzymatic reactions undergoing classification and the grouping of similar reactions together into more refined clusters or subclasses.

This leads to the second criteria on a metaphysics of classification of chemical reactions. In order to be descriptively fit for purpose a metaphysics must permit the identification of relevant similarity relations since it is these similarity relations on which the classification of reactions is built. It must provide a framework for classification that is able to support predictions about the behaviour of reactions on the basis of the similarity relations identified in the classification. This criterion is crucial since it enables the formulation of predictions regarding the behaviour of chemical reactions and thus makes the classifications useful for the sort of industrial and medical applications discussed in section 2.1. The kind of similarities that need to be accommodated by our metaphysics when making predictions are as follows;

1. Reactions falling in cluster A are disposed to increase in speed in the presence of enzyme X
2. Reactions falling within cluster B are disposed to begin reacting in the presence of activation energy Y
3. Reactions in cluster C are all disposed to speed up in the presence of certain environmental conditions concerning temperature, pressure and concentration.

In addition to these common statements regarding how a reaction will proceed there is another variety of similarities that need to be accommodated in our metaphysics. These are those are revealed by the classification of enzymatic reactions and are shared by the members of a particular subclass or cluster;

1. Number of bonds broken during the reaction
2. The change in bond order i.e. single bond converted to double bond
3. The consecutive Vs simultaneous breaking of bonds
4. Substructure of the reaction i.e.
    a. Part of the entity of which the reaction is centred
    b. Substances released during the reaction in addition to the desired product

A metaphysics for the classification of chemical reactions must have the resources to capture all the similarities listed above. This is essential for a metaphysics that is descriptively fit for purpose because predictive statements are made on the basis of these similarity relations. Reactions appearing close to each other on the reaction landscape will exhibit a strong similarity relation which chemists have learnt through experience that these are capable of supporting predictions. For example, which enzymes will catalyse which reactions and under what amount of activation energy. If a particular metaphysical framework is unable to capture these similarity relations then chemist's ability to make successful predictions will be reduced.

The criterion of similarity is linked to a further debate within the metaphysics of science. I previously discussed the issue of capturing similarities in chapter 1, when I addressed the debate surrounding whether ontological commitment to natural kinds is required in addition to commitment to properties. Those who reject commitment to natural kinds commonly argue that kinds are redundant because the sorts of similarity they are introduced to ground can be adequately captured by properties. Armstrong, for instance, argued that the job of capturing similarities is done by sparse properties.

> 'Sharing of [the sparse properties] makes for qualitative similarity, [the sparse properties] carve at the joints, they are intrinsic, they are highly specific, the sets of their instances are ipso facto not entirely miscellaneous, and there are only just enough of them to characterize things completely and without redundancy' (Armstrong, 1986, 60).

More recently in his paper *Two Conceptions of Sparse Properties* Schaffer (2004) adjudicates a dispute between a scientific conception of sparse properties in which they are found at all levels of scientific discourse and the fundamental conception in which sparse properties equate with fundamental properties. His preference for the scientific conception of sparse properties stems from the need to ground objective similarities appearing at higher levels of inquiry such as at the psychological, neurobiological, and chemical levels.

This debate between kinds and properties will play an important role throughout the rest of my thesis as I examine whether ontological commitment to reaction is required to capture the similarities revealed in classification or whether they can be accommodated through a commitment to properties alone. I will discuss this issue extensively in chapter 4.

### 2:5:3: Explanatory Unification

Thirdly I argue that a metaphysics is descriptively fit for purpose if it is able to capture the similarity relations between reactions that result from classification and incorporate them into the broader framework of chemical knowledge. This promotes a better understanding of reactions and furthers the fruitful development of science. This leads to the third general requirement on our metaphysics; that it promotes explanatory unification.[12]

The idea is that by incorporating the similarities revealed by the classification schemes into existing chemical knowledge, chemists are better able to understand and explain the behaviour of reactions and to better manipulate this knowledge in the future. Thus explanatory unification supports and promotes the fruitful development of chemistry.

Explanatory unification is a theme that runs throughout the classification process. Consider again the methodology behind the use of QSAR discussed in

[12] I note that this is a controversial requirement that stems from my approach of identifying a metaphysics that best meets the needs of practice.

section 2.4. The aim was to achieve a more refined classification of reactions by unifying the relevant structural properties with the macro level activities they are responsible for producing. The importance of unification can also be seen in the resulting 2 -dimensional reaction landscape. At the beginning of this chapter I discussed the idea that chemists employ neural networking in order to mirror the concept of a reaction map had by chemists in which they mentally store and organise reaction information. The 2-dimensional scheme is adopted because chemists want a better, more unified understanding of the way in which the different types and sub types of reactions relate to one another rather than a specification of types and a list of corresponding tokens. This promotes the fruitful development of science and allows for the formulation of further more accurate predictions as discussed in the previous section.

Gasteiger states that the 'classification of enzymatic reactions is a field of great interest as data on proteins with unknown function grows fast and the modelling of biochemical reaction networks depends on the knowledge of protein functions' (Gasteiger, 2007, 1526). Thus even if the classification systems previously described reveal similarities that do not necessarily lead directly to greater predictability it is still important that our metaphysics provides a framework in which they can be incorporated into our body of scientific knowledge. If a metaphysics is to be compatible with the classification of chemical reactions it must provide the resources for explanatory unification and in particular, be able to explain why these objective similarities hold and why they are successful in supporting predictions.

## 2:5:4: Minimalism

The final requirement on our metaphysics is that it is minimal, i.e. it provides the smallest, most basic account of all the things in the world whilst still meeting the basic criteria for adequacy. In debates over the metaphysics of classification minimalism has traditionally been balanced against strength and the desire to capture similarity. For example, as I discussed in chapter 1, Lewis and Armstrong cite concerns over minimalism when rejecting commitment to natural kinds whilst Ellis

sacrifices concerns over minimalism by postulating his three hierarchies of natural kinds. Schaffer outlines the role of the minimalist requirement as follows;

> 'The project of providing a minimal ontological base is part of the project of providing an ontological assay. The goal of an ontological assay is to characterize the contingent basis for all contingent truths. Suppose that there are fundamental properties on which the macroproperties supervene. Then these fundamental properties are perfectly suited to serve as a minimal ontological base. Specify which fundamental properties are where, and the arrangement of the macro-properties is thereby fixed' (Schaffer, 2004, 94).

Schaffer's point is that if higher level properties supervene on lower level properties then commitment to higher level properties is not required since, their existence is already fixed by lower level properties. This supervenience relation is asymmetrical, i.e. if we are ontologically committed to higher level properties this does not necessarily fix the existence of lower level properties.

My project is to provide the most appropriate metaphysics for the classification of reactions in practice. This metaphysics will best meet the criteria of descriptively fit for purpose by being descriptively accurate enough, capture similarity relations and enhance explanatory unification. I suggest that the criterion of minimalism is relevant to my project in two scenarios, if

a. Two ontological accounts of classification were equally successful in which case we should prefer the one that has the more minimal resources
b. An ontology becomes so inflated that this inhibits its ability to successfully meet the other criteria

Since neither of these eventualities occur in my thesis, discussion of the criterion of minimalism will be limited.

I take these criteria on a metaphysics for classification of reactions to be intimately related. Descriptively fit for purpose provides a general criterion in which the other criteria fall. For instance, descriptive accuracy in the relevant respect is required to capture the similarity relations that hold between the reactions undergoing classification. In addition, a metaphysics is only descriptively fit for

purpose if chemists are able to use the reaction landscape in order to capture similarities. This is required for formulating successful predictions and therefore advancing the fruitful development of science. Finally the criteria of explanatory unification also falls within the scope of descriptively fit for purpose. Placing the knowledge regarding similarity relations that results from the reaction landscape within the context of existing chemical knowledge will enhance chemists' ability to produce additional classificatory schemes using QSAR and make successful predictions on this basis.

## 2:6: Conclusion: Initial Implications for a Metaphysics of Classification

The aim of my thesis is to provide an appropriate metaphysical account for the classification of reactions in practice. In chapter 1 I outlined different approaches to the philosophy of classification and the status attributed to natural kinds in each case. I showed that these accounts were focused on the classification of entities and their application to the classification of 'non-entity like things' had not been explored in detail.

The aim of this chapter has been to examine a new methodology for the classification of reactions in practice and to draw from this a set of criteria that will be used throughout the rest of my thesis to adjudicate between different ontological frameworks. A metaphysics of classification must adhere to these criteria if it is to be compatible with classification in practice.

I began in section 2.1 by discussing the context of my case studies and the development of chemoinformatics as a new discipline, emphasising its importance in industrial applications of chemistry. In section 2.2 I outlined a new methodology for the classification of reactions focusing on the use of QSAR and neural networking. I showed how it was applied as a test case to the classification of organic reactions with a high degree of success with classification schemes having large information content. In section 2.3 I focused specifically on the methodology of classification and

drew out some initial requirements on a metaphysics for the classification of reactions. Firstly, I argued the methodology is primarily used for refining existing classifications and so must be compatible with other methods that produce the initial classification scheme. Secondly, I argued that we must treat activities as heuristics for classification and outlined the implications of this for the debate between whether classification should take place at the micro or macro level in chemistry. Thirdly, I discussed the implications of representation in classification and the advantages of a 2-dimensional classificatory scheme.

In section 2.4 I discussed a more recent application of the methodology to the classification of enzymatic reactions and in section 2.5 I related this to three more general requirements on a metaphysics of classification; it must be *descriptively fit for purpose*. This amounts to being *descriptively accurate 'enough'* to meet the aims of inquiry, being able to *capture the similarity relations between reactions* and *promoting explanatory unification*.

On the basis of the discussion so far in this chapter I can makes some initial comments on which accounts of classification outlined in chapter 1, best describe the status of the types of reactions that result from this classification. Firstly I suggest that we can rule out social constructivism as appropriate to accommodate the kind of classification going on in my case study. QSAR and neural networking came to prominence due to demands from industry for greater predictability and manipulability of chemical information. QSAR and neural networking are employed because they provide a methodology for systematising and organising large volumes of data in such a way that permits successful inductive inferences. For example, in the case of enzymatic reactions discussed in section 2.4 the resulting classification scheme was used to better predict which enzymes would catalyse which reactions and under what conditions.

This allows us to rule out social constructivism by appealing to the no miracles argument; the best explanation of the success of predictions is that the similarity relations revealed by QSAR and neural networking are real and capture the real similarity relations that exist in nature. In addition the classification is not produced

for the sake of classification itself but to gain a better understanding of a particular chemical phenomenon and to make successful predictions. In so far as the investigation is non-objective and lead by human interests, this is because is directed specifically towards a better understanding of this phenomenon. This suggests that a realist account of classification is most appropriate but we still must adjudicate between the varieties of weak realism and the stronger essentialist positions discussed in chapter 1.

I suggest there is reason to reject the stronger versions of essentialism on which natural kinds have essences. The classification process is led by the scientific aims and interests of the chemists conducting the investigation and is therefore subject to perspectivalism. It is conceivable that chemists investigating a different chemical problem would have classified the reactions differently. For example, the similarity relations revealed on the reaction landscape are relative to the reactions undergoing classification. If more reactions are input into the system then this will alter the extent to which any two reactions are deemed to be similar to each other. In addition, when classifying in practice chemists do not take reactions to have essential properties but take their instantiation to correlate with the presence of certain physicochemical properties of the reactions centres of entities.

Instead we are left with weak realist accounts of natural kinds, such as Boyd's homeostatic property cluster kinds, Dupré's promiscuous realism and Hendry's microstructuralism. Each of these positions appeals to a range of different ontological components such as entities, properties, mechanisms and processes. In order to establish which account should be adopted for the classification of reactions I need to establish which of these components we must be ontologically committed to in order to capture the classification of reactions. I will be primarily concerned with this question through the course of the next three chapters. I will then assess the implication of this discussion for the natural kind debate in chapter 6.

Since the classification of reactions takes place on the basis of physicochemical variables that best describe how a given reaction mechanism will proceed, a sensible place to start is with the literature on mechanisms in the

philosophy of science. I will focus on the account of mechanisms given by Machamer, Darden, and Craver and assess whether their entities and activities ontology is sufficient for capturing the classification of chemical reactions in practice.

# *Chapter 3: Can the Entities and Activities Ontology capture the Classification of Reactions in Practice?*

## 3:1: Introduction

The aim of my thesis is to identify the most appropriate metaphysics to accommodate the classification of chemical reactions in practice. I began in chapter 1 by outlining the literature on natural kind classification and arguing that it cannot straightforwardly accommodate the classification of reactions. In chapter 2 I discussed the classification of chemical reactions in practice and used this to draw out a number of requirements that any metaphysical framework must be compatible with if it is to accommodate the classification of reactions in practice. I argued that this discussion of practice revealed that constructivist and strong essentialist theses were unable to capture the metaphysical status of types of reaction. I also suggested that to adjudicate between other varieties of weak realism we needed to investigate which ontological components are required to accommodate the classification of reactions. The remaining accounts of natural kind classification refer to components such as entities dispositional properties, mechanisms or processes.

My discussion of chemical practice revealed the concept of a reaction mechanism to be central to understanding the nature of chemical reactions. In chapter 2 I showed how reactions were classified on the basis of properties that were thought to reveal similarities in these reaction mechanisms. As a result, in this chapter I will address the metaphysics of mechanisms. I will address whether this ontology is sufficient to capture the classification of reactions in practice.

I will focus on the account of mechanisms provided by Machamer, Darden and Craver (MDC) in their 2000 paper *Thinking about Mechanisms*. Whilst other related accounts of mechanism have been provided by *Glennan 2002* and *Bechtel and Abrahamsen 200*5, I will focus only on the account provided by MDC since it is only they who introduce the notion of activities alongside entities and as I have shown in chapter 2 activities are central to chemical practice when classifying reactions.

The aims of this chapter are two-fold, firstly I will engage in an interpretive project drawing out and developing key ideas proposed in their paper *Thinking about Mechanisms (2000).* Whilst the paper motivated a productive literature on the notion of mechanisms in science, very little has been said on the metaphysics of activities. This is with the exception of Illari and Williamson (2013). The project of fleshing out what is meant by an activity will proceed throughout the course of this chapter as questions arise with respect to activities and modality, actuality and the relation of activities to properties.

On the basis of this interpretive work, I will address whether the entities – activities ontology is sufficient to accommodate the classification of chemical processes in practice. This discussion will take place within the context of the criteria outlined in chapter 2 which required that our metaphysics be descriptively fit for purpose; i.e. descriptively accurate, capable of capturing similarity relations and promoting explanatory unification.

I will begin in section 3.1 by providing an account of MDC's entities – activities ontology and placing it within the context of the wider literature on mechanisms. In section 3.2 I will discuss the use and meaning of the term 'activity' within the chemical literature. This will allow for a comparison of the use of the term 'activity' by chemists and philosophers. In section 3.3 I will refer back to the case specific requirements outlined in section 2.3 and raise some initial concerns regarding MDC's account. In section 3.4 I will discuss whether the entities – activities ontology is capable of meeting both case specific and general sets of requirements.

I will conclude that the entities – activities ontology fails to meet the criteria of capturing similarity relations because it lacks the modality required to capture predictive statements. I argue that one option is to give a modal reading of activities however I suggest that activities lack the required sort of potentiality for this to be a viable option. The other option is that MDC implicitly commit to dispositional properties. Even if they choose this second option I argue that to play down the role of dispositional properties by referring to their account as a two category ontology of activities and entities violates the criteria of explanatory unification and descriptive accuracy. Since the entities – activities ontology does not meet the three criteria of capturing similarity relations, descriptive accuracy and promoting explanatory unification, it is therefore not descriptively fit for purpose with respect to my case study.

## 3:2: Activities in the Mechanism Literature

In this section I will focus on the account of mechanisms provided by Machamer, Darden and Craver (MDC) in their 2000 paper *Thinking about mechanisms.* More specifically, I will provide an examination of the term 'activity' as it is used in the mechanisms literature. I will then discuss the work of Illari and Williamson who have offered an analysis and defence of MDC's activities, they also flesh out discussion by (Machamer 2004) who addresses but doesn't not further develop discussion of activities in (MDC, 2000) . Little else has been said about activities, so there is significant work to be done if I'm to assess whether entities and activities are able to accommodate classificatory practice.

Along with acquiring a better grasp of the notion of an activity, the second purpose of this exegesis is to allow for a comparison between the way the term 'activity' is used by philosophers and the way it is used by chemists engaged in the classification of chemical reactions. If they are using the term in a consistent way, then it is legitimate for me to use the latter as a test case for the former.

MDC's aim is for their account to be descriptive of actual scientific practice. Whilst their examples are taken from molecular biology and neurobiology it is hoped their account will be applicable to other scientific domains such as chemistry. MDC claim that 'mechanisms are entities and activities organized such that they are productive of regular changes from start or set- up to finish or termination conditions' (Machamer, Darden and Craver, 2000, 3).

The mechanism runs from start to end such that the product of the mechanism arises as a result of the start conditions and intermediate phases. Mechanisms are composed of entities and activities and when these components of the mechanism are ordered correctly it will be productive of regular change. For MDC examples of entities include 'cell membrane , vesicles, microtubules, molecules and ions,' whereas examples of activities include 'biosynthesis, transport, depolarization, insertion, storage, recycling, priming, diffusion, and modulation' (Machamer, Darden and Craver, 2000, 8).

MDC's paper focuses on entities and activities and takes these to be independent components that work together to bring about change via a mechanism. Nonetheless, they hint at a place for properties within their ontology. They state for instance that 'mechanisms are composed of both entities (with their properties) and activities' (Machamer, Darden and Craver, 2000, 3). However they do not provide significant elaboration on the nature of these properties or their status within their ontology. They do state that; 'activities usually require that entities have specific types of properties. The neurotransmitter and receptor, two entities, bind, an activity, by virtue of their structural properties and charge distributions' (Machamer, Darden and Craver, 2000, 3).

This suggests at the least their ontology should contain structural properties. They do not pass comment on whether ontological commitment to dispositional properties or capacities is required in addition. Throughout the course of this chapter I will suggest that MDC ought to commit to dispositional properties, in addition to entities and activities, in order to accommodate the classification of reactions as

outlined in my case study. I will return to MDC's discussion of properties in section 3.6.5.

MDC's account is dualistic since they ascribe equal ontological significance to the activities and entities that constitute the mechanism. MDC intend is to capture the best of substantival ontologies that reserve ontological commitment to entities and properties and the best of process ontologies that reserve commitment only for processes. On the MDC view entities are taken to be the things that engage in activities and activities are types of change. They must both be correctly positioned within the mechanism in order for the mechanism to function correctly (Machamer, Darden and Craver, 2000, 2).

On the substantivalist view to which MDC refer, typically change occurs as a result of entities manifesting their capacities. For instance, DNA bases are entities that undergo change by manifesting their capacities such as their weak polarities or their charge configurations. However it is argued by MDC that an entity based ontology such as this is insufficient. They outline at least two reasons for this.

Firstly, according to MDC activities are conceptually prior to capacities, since one must have an idea of the activities that are possible before one can ascribe the capacity to engage in that activity to a relevant entity. MDC give the example of aspirin's ability to cure a headache, they state; 'one does not know that aspirin has the capacity to relieve a headache unless one knows that aspirin produces headache relief' (Machamer, Darden and Craver, 2000, 5). Secondly, MDC argue that by focusing only on entities and capacities such ontologies neglect the fact that mechanisms are 'active' and are subject to scientific investigation in their own right. MDC prefer to characterise change in terms of mechanisms rather than asserting that change is just a change in the properties of an entity (Machamer, Darden and Craver, 2000, 6).

In contrast to substantivalist approaches, MDC describe activities as the 'producers of change', they bring about changes in the relevant entity and in this sense can be thought of as causes (Machamer, Darden and Craver, 2000, 6). Whilst

an activity is characterised as a type of cause, MDC buy into an Anscombean account of causation whereby they prefer to treat 'cause' as an abstract term that can be filled in by the relevant activity as it is specified in scientific theory (Machamer, Darden and Craver, 2000, 6). They do not flesh out the notion of activities as causes any further, they do however, give more details on the characteristics of activities.

Firstly they assert that activities are temporally extended and dynamic rather than static, they are 'active kinds of changing' (Machamer Darden and Craver, 2000, 5). MDC's discussion of how activities can be identified reveals that they can be exist at different levels and can described in various levels of detail depending on the contextual requirement. It's claimed that;

> 'activities, likewise, may be identified and individuated by their spatiotemporal location. They also may be individuated by their rate, duration, types of entities and types of properties that engage in them' (Machamer, Darden and Craver, 2000, 5).
>
> 'More specific individuation conditions may include their mode of operation (e.g., contact action versus attraction at a distance), directionality (e.g., linear versus at right angles), polarity (attraction versus attraction and repulsion), energy requirements (e.g. how much energy is required to form or break a chemical bond), and the range of activity (e.g., electro-magnetic forces have a wider influence than do the strong and weak forces in the nucleus)' (Machamer, Darden and Craver, 2000, 5).

Activities may be given a lower level mechanistic description in terms of other entities and activities whilst being correctly considered activities in their own right and themselves functioning in higher level mechanisms.

Whilst it is argued that activities possess the same ontological status as entities, they should not replace entities altogether. This is because, according to MDC, activities are always 'of entities.' At least within the domains of molecular biology and neurobiology that are discussed, MDC know of no activities that exist independently of entities. Entities and activities are ontological components that are interdependent in practice. The nature of the activity determines what kinds of properties are able to take part in that activity whilst the properties of entities determine what activities they're able to engage in.

MDC do not offer any further insight into the nature of an activity and activities have received little attention in the wider mechanism literature. This is with the exception of the discussion by Illari and Williamson in their paper *In Defence of Activities* (2013). Illari and Williamson further explore the notion of activities as described by MDC and offer a comparison of the entities - activities ontology with the entities – capacities ontology which they deem to be its closest rival. The aim of their discussion is to begin a debate regarding the status of activities; they do not comment on whether an activities – entities ontology is itself sufficient without additional commitment to capacities.

Illari and Williamson argue that activities are prior to capacities epistemically and conceptually. To take the epistemic point first, it is argued that we cannot know that an entity has the capacity to engage in a given activity until we have observed it engage in that activity. I referred to this point earlier when discussing MDC's claims that we cannot know that aspirin has the capacity to offer pain relief until we have seen it do so. This epistemic consideration is given more force with the addition of a conceptual argument offered by Machamer stating that 'activity must precede potentiality,' (Machamer, 2004 30). Illari and Williamson agree with his point is that we must have the concept of an activity prior to the concept of a capacity because to say that an entity has a capacity is to say it has a capacity to engage in an activity, therefore we must have the concept activity prior to the concept capacity (Illari and Williamson, 2013, 16).

Illari and Williamson also agree with MDC that activities are extended in time and constitute types of change. However they point to a further difference between activities and capacities concerning arity. They suggest activities can be distinguished from capacities because they have unrestricted arity, whilst capacities can only have a one to one arity. An activity can be associated with as many entities as necessary while capacities can only attach themselves to one entity. It is argued that this unrestricted arity allows the entities - activities ontology to promote scientific understanding since it offers a more appropriate description of nature. For instance, Illari and Williamson argue that certain phenomena such as osmosis are better

understood when viewed holistically as one activity rather than reduced to the capacities of different entities. When the phenomena is described in this way we have a more appropriate starting point for scientific investigation allowing for a better understanding of the factors affecting the activity, how it might behave differently with different entities partaking in it and how to manipulate it to produce desired effects. I will discuss the issue of arity in more detail in section 4.4.

Illari and Williamson also refer to the way in which activities and capacities are referred to in ordinary discourse. They discuss cases from evolutionary theory, biology, chemistry and physics and suggest that in each case activities are referred to in a way that is distinct from entities and capacities. In the case of chemistry, Illari and Williamson describe how activities are classified independently from the molecules that take part in them. They give the example of reaction mechanisms $S_n1$ and $s_n2$ where the first refers to substitution nucleophilic unimolecular reactions whereas $s_n2$ refers to substitution nucleophilic biomolecular reaction. Both of these reaction have a common structure which means that examples are identified regardless of the type of entities engaged in the reaction. It seems that science does reveal things that are not entities or capacities but which have 'unrestricted arity in their relation to entities' and which are 'extended in time' (Illari and Williamson, 2013, 8). Illari and Williamson conclude that a descriptively adequate ontology must include a separate ontological category for activities.

They go on to further develop the account provided by MDC. They state that if ontological commitment to activities is required then we must limit what sorts of activities should fall in this category. They argue that we should distinguish between those activities that are present in everyday life such as the clockwise spinning of spinning tops and those activities that appear in mechanisms such as the $S_n1$ reactions. Those activities that appear in mechanisms are characterised by a certain level of stability and repeatability, such that regardless of the entity that is taking part in the activity the activity will exhibit a continuity in its characteristics. Much the same idea applies to entities; those entities that appear in mechanisms must be stable enough such that when working in conjunction with another relatively stable activity

they will be productive of a phenomenon in a regular and repeatable manner (Illari and Williamson, 2013, 1). It is intuitive to require that activities have a degree of stability in order to function in mechanisms however there are many highly stable activities such as the tying of shoe laces that do not constitute scientific mechanisms. I shall refer to this point in section 3.5.5.

## 3:3: Activities in the Classification of Chemical Reactions

In section 3.2 I discussed the place of activities within the entities - activities ontology and drew out their key features. In this section I will discuss those activities referred to by chemists working within the domain of chemoinformatics discussed in chapter 2. I'm interested in what chemists have in mind when they use the term 'activity'. If their definition of activities concurs with MDC, then we can use examples from the domain of QSAR to assess the adequacy of the entities – activities ontology. If the two definitions do not coincide then we must question the extent to which the MDC account is representative of scientific practice and suggest modifications to their account.

In chapter 2, I discussed the classification of reactions in practice and drew out various criteria that a metaphysics must adhere to if it is to be compatible with this element of scientific practice. I described the importance of identifying a QSAR for reactions when producing a classification of chemical reactions where the purpose of QSAR is to identify a relationship between lower level structural properties and a higher level activity (or reaction)

Once a relationship has been identified it is used to make predictions about future occurrences of that activity since QSAR is based on the assumption that lower level structural similarity gives rise to a similarity in higher level activities. We know from the discussion of QSAR in chapter 2 that the 'S' in QSAR refers to the structural properties that describe the reaction centre i.e. the properties of those atoms and bonds that undergo change during the reaction, since the properties of the reaction centre will be indicative of the type of change that will occur. How to fill in the term

'activity' changes depending on what the chemist is interested in. In the classification of reactions, the activity is the occurrence or instantiation of a particular type of reaction. Chemists identify those structural properties that are associated with the instantiation of that particular reaction. We know then, that for chemists, activities are types of reactions where reactions are things that can be made to undergo instantiate.

We should also note the aims and interests of chemists investigating the things they refer to as activities. These might include;

- The prediction of a variety of physicochemical properties of molecules (whether they be pharmaceuticals, pesticides, personal products, fine chemicals, etc.).
- The prediction of the fate of molecules which are released into the environment.
- The rationalization and prediction of the combined effects of molecules, whether it be in mixtures or formulations.
- The prediction of toxicity to environmental species.
- The rational identification of new leads with pharmacological, biocidal or pesticidal activity' (Consonni and Todeschini, 2010, 4).

This suggests the importance of the need to study activities as distinct beings in their own right, in order to better understand the factors that affect them and the ways in which they behave when different entities are engaged in them. I suggest this is the first similarity between chemists' approach to activities and the account provided by MDC. Both attribute a high status to activities such that they are worth studying in their own right and not just reducible to entities.

Secondly I suggest both chemists working on QSAR and MDC take activities to be kinds *of change*. In the case of chemical reactions this involves some change in the entities involved in the reaction whereby the classificatory output groups these changes into similar types. We can see this by referring back to the three stage classification process outlined in chapter 2. In order for classification by QSAR and neural networking to take place, a preliminary classification of reactions into general types of changes in entities must have taken place. This is then further refined to

identify the subtypes of reactions within that type. In the case of the classification reactions, the activity of interest was hydrolysis reactions.

Activities also have the property of being extended in time, chemical reactions are non – instantaneous and so are the other activities described in this section. For example, toxic chemicals take a period of time to infect nearby entities and systems whilst the dissolution of water in solution takes time to unfold. This is supported by the fact that the reaction mechanisms referred to in the discussion of enzymatic reactions involve multiple steps in which the first step must take place before the second. I will discuss the extension of reactions in time in section 4.1.

Finally each activity or reaction is associated with at least one entity and tends to involve many more. In section 1.2 I made a distinction between a reaction and a reaction mechanism. A reaction mechanism involves at least two entities and potential intermediate entities. However a reaction itself will involve many instantiations of the reaction mechanism. To take a more familiar example, the dissolution of sugar in tea involves many sugar molecules and many molecules of water, each of which will undergo the action of dissolution. An explanation of why stirring the tea increases the rate of dissolution requires an account of the probability for collisions and therefore reference to the many entities involved in the dissolution process.

More generally, proponents of QSAR and MDC agree on their approach of working by examples rather than giving a definition of what constitutes an activity. I suggest that MDC would be happy to accept chemical reactions as an example of an activity; a reaction is an instance of change that is engaged in by entities, the reaction is extended in time, and can be given a characterisation in terms of a lower level mechanism. Since MDC would accept chemical reactions as a type of activity and since QSAR is an example of classifying activities in practice, whether or not an entities – activities ontology is sufficient to accommodate this case study constitutes a good test of the ontological framework.

# 3:4: Initial Cause for Concern

## 3:4:1: Preliminary Concerns

Thus far in this chapter I have explored the entities – activities ontology proposed by MDC and have reviewed some initial arguments why ontological commitment to activities should be taken seriously. I went on to evaluate the use of the term 'activities' in the chemical literature and concluded that MDC would accept the activities identified in QSAR as constituting examples of activities on their account.

I can now begin to address the question of whether an entities – activities ontology is sufficient to capturing the classification of chemical reactions in practice. The purpose of this section is to give a reminder of the case specific criteria outlined in section 2.3 and indicate some initial reasons to doubt whether these can be met. A more conclusive argument will follow in section 3.5 in which I further discuss these requirements with respect to the general criteria on our metaphysics outlined in section 2.5 that must be met if a metaphysics is to be descriptively fit for purpose i.e. descriptive accuracy, capturing similarity relations and explanatory unification.

In section 2.3 I noted some initial features of chemical practice that a metaphysics of classification must be compatible with.

a. The classification of reactions is a three stage process; firstly a type of reaction is identified using theoretical knowledge, secondly, a more refined classification of this type of reaction is produced using QSAR and thirdly a representation is constructed using neural networking

b. The output of classificatory schemes is represented on a 2-dimentional reaction landscape. Chemists use this representation when making predictions rather than appealing to traditional 1 -dimensional categories such as 'carbon' 'oxidation reaction' etc.

c. The properties on which the classification of reactions is based take the form of physicochemical descriptors of the reaction

d. The aim of classification is to provide a unified account of microstructural and macro level properties

The first two criteria are not obviously problematic for the entities – activities ontology. For example, I described in section 2.2 how the classification of reactions takes place through the representation of a reaction landscape on which the relations between reactions can be identified. This is compatible with taking reactions to be activities whereby it is the relations between activities that are represented. It is also compatible with criterion c. the three stage classification process described above. This is because MDC are open to the possibility that a particular activity can be divided into sub types of activities which can in turn be given a more fine – grained description that reveals more subtle similarities.

It is the final two constraints that may be problematic for the entities - activities ontology. In what follows I will spell out initial reasons to doubt whether such an ontological framework is able to accommodate these criteria and begin to hint at the worry that an additional ontological category of dispositions is also required.

The problem concerns how to accommodate the use of physicochemical properties with the entities – activities ontology. These properties are required for giving a unified account of activities (criterion d) which can then be used as the basis for classification (criterion a). The difficulty is that these properties are not straightforwardly accommodated on the entities – activities ontology and first impressions indicate they are better characterised as dispositional properties. As I have previously hinted, it is not clear how dispositions are accommodated on the entities – activities view.

Consider the property inductive effect; this property was used to encode reactions in both the case studies described in chapter 2. In particular, chemists were

interested in the inductive effect associated with the atoms that make up the reaction centre. It is defined as a measure of the transmission of the polarising effect of an electronegative atom through a chain of atoms in a molecule. 'The polarising influence of an electronegative atom decreases with the number of intervening sigma bonds. This is called the inductive effect. It is generally accepted that the inductive effect is attenuated by a factor of 2-3 by each intervening bond' (Gasteiger, 2009, 176).

Now consider the molecule $C_2H_4CL$. The chlorine's electronegativity means its electrons are not equally shared between the chlorine and carbon but are dragged towards the chlorine. This means that the carbon is left with an electropositive charge and so drags the electrons in the next nearby carbon closer towards it in order to gain a bigger share of the electrons. This unequal sharing of electrons continues along the chain of molecules but to a smaller extent with each degree of separation from the original source of the electronegativity. The overall distorted shape of the molecule is a result of the inductive effect.

If inductive effect is a measure of polarizing influence which is in turn a measure of electron attracting power then it is not obvious that taking inductive effect to be an activity is the most appropriate characterization. In what follows I will examine what a characterization of polarity as an activity looks like and then examine what a characterization of polarity as a disposition looks like. This will set up discussion in the following section in which I examine which characterization is most appropriate.

## 3:4:2: Polarity and Inductive Effect as Activities

There are two ways in which we can characterize inductive effect as an activity according to MDC. The first sense builds on the idea that mechanisms are hierarchical. The second treats a mechanism as non-reductive. It's claimed that; 'Mechanisms occur in nested hierarchies and the descriptions of mechanisms in

neurobiology and molecular biology are frequently multi-level'(Machamer, Darden and Craver, 2000, 13).

On the hierarchical view the activities that constitute a given mechanism can be specified in terms of a lower level mechanism. For instance when describing the mechanism by which chemical signals are transmitted across a synapse, MDC suggest that the activities involved such as biosynthesis, depolarization, and transport are further specified in terms of a lower level mechanism.

I described above how inductive effect and polarity result from an unequal sharing of electrons. We can describe the activity inductive effect in terms of the lower level mechanism illustrated below and described with the following steps.

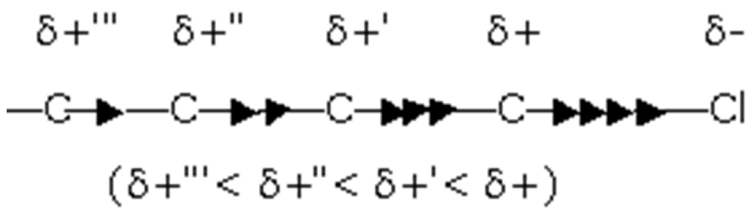


*Figure 17: an illustration of Inductive Effect*

The chlorine atom engages in the activity of attracting the shared pair of electrons from the carbon atom next to it leaving the carbon atom with a positive charge. As a result the carbon atom engages in the activity of attracting electrons from the next carbon along in order to partially neutralize its positive charge. This in turn causes a positive charge on the next along carbon molecule which also engages in the activity of attracting a carbon atom and the mechanism continues along the chain of atoms. Each activity brings about a change in the next atom.

MDC stop short of implying that all activities can be specified in terms of a lower level mechanism and assert that there are some activities for which no lower level description can be given.

> 'Higher-level entities and activities are thus essential to the intelligibility of those at lower levels, just as much as those at lower levels are essential for understanding those at higher levels. It is the integration of different levels

> into productive relations that renders the phenomenon intelligible and thereby explains it' (Machamer, Darden and Craver, 2000, 24).
>
> 'In molecular biology and molecular neurobiology, hierarchies of mechanisms bottom out in descriptions of the activities of macromolecules, smaller molecules, and ions' (Machamer, Darden and Craver, 2000, 14).

In addition, there may be activities that are awaiting specification in terms of lower level mechanisms, there is no reason to deny that these constitute activities even if they are not bottom out activities.

Within the remit of molecular biology and molecular neurobiology MDC isolate four categories of bottom out activities: geometrico-mechanical electro-chemical; energetic and electro-magnetic. It is electrochemical that are most relevant to present purposes, these are described as

> 'Attracting, repelling, bonding, and breaking are electro-chemical kinds of activity. Chemical bonding, such as the formation of strong covalent bonds between amino acids in proteins, is a more specific example. The lock and key docking of an enzyme and its substrate involves geometrical shape and mechanical stresses and chemical attractions' (Machamer Darden and Craver, 2000, 14).

Even if we can infer from the discussion above that a specification of inductive effect in terms of a lower level mechanism cannot be given either for epistemic reasons or because it is a bottom out activity then it must still be a producer of change and be engaged in by entities. I previously suggested we should read MDC as implying that the 'doings' of activities are extended in time. This reading is further supported by the claim that activities can be individuated by their spatiotemporal location as well as their rate and duration, again, requiring their extension in time.

If something meets these criteria then there is good reason to suppose it can be characterized as an activity. Inductive effect certainly brings about a change, the overall change is a distortion in the shape of the molecule due to the unequal sharing of electrons. This change is non instantaneous and is extended in time. Inductive effect has a spatial-temporal location and it occurs between the atoms that engage

in it. Therefore it satisfies all four points and it seems plausible that inductive effect can be characterized as an activity in either of the senses alluded to by MDC.

### 3:4:3: Polarity and Inductive Effect as Dispositions

I have shown above that inductive effect can be reasonably accounted for by treating it as an activity. I will now show that polarity can also be reasonably accounted for in terms of dispositional properties. To flesh this out I will appeal to Chakravartty's notion of a causal process and attempt to account for inductive effect in terms of the transference of dispositional properties. Chakravartty's approach to causal process stems from his desire to give an account of causation. He argues that the true relata of causation are not events but causal process in virtue of the causal properties that constitute these processes. He defines a causal property as 'one that confers dispositions on the particulars that have it to behave in certain ways when in the presence or absence of other particulars with causal properties of their own' (Chakravartty, 2007, 108).

He gives the examples such as mass where bodies that possess mass will be disposed to accelerate when experiencing a force. Likewise, gases with different volumes will be disposed to vary in temperatures when exposed to different pressures. On Chakravartty's view we can think of causal processes such as the inductive effect as resulting from the continuing manifestation of such dispositional properties. The manifestation of one property provides the stimulus conditions for the manifestation of many other dispositional properties which in turn stimulate the manifestation of a web of additional dispositional properties leading to the 'continuous flux of causal activity' to which Chakravartty refers (Chakravartty, 2007, 108).

In the case of inductive effect we can give an account of the phenomena by isolating the relevant dispositional properties involved in bringing about the desired effect from the wider causal web that forms its context.

a. The chlorine atom's disposition to attract neighbouring electrons

b. The carbon$_1$ atom's disposition to retain a partial hold of its electrons (and neutral charge)
c. The carbon$_1$ atoms disposition to re-establish its neural charge by attracting electrons from neighbouring carbon$_2$ atoms.
d. The carbon$_2$ atom's disposition to retain a partial hold of its electrons (and neutral charge)
e. The carbon$_2$ atoms disposition to re-establish its neutral charge by attracting electrons from neighbouring carbon$_2$ atoms.
f. The carbon$_1$ atom, carbon$_2$ atom and carbon$_3$ atoms dispositions to attract and electron from hydrogen
g. The Hydrogen$_1$ atom and Hydrogen$_2$ atom and Hydrogen$_3$ atom's disposition to retain their share of the electron.

Inductive effect is then characterized as the coming together of these overlapping dispositional properties.

I have described above how the physicochemical property 'inductive effect' might be characterized in terms of dispositional properties and how it might be characterized in terms of an activity. In the next section I will examine which account is most descriptively fit for purpose.

## 3:5: Problems with the Entities and Activities Ontology

The aim of this section is to build on the discussion in the previous section and examine whether the activities – entities ontology can capture the classification of reactions without additional commitment to dispositional properties. Given the lack of discussion in the literature on the nature of activities, much of this project is interpretive and requires me to outline what we should want activities to be able to do if they are to be compatible with chemical practice. I will then address whether this is possible given what MDC say about activities.

It is worth clarifying that the aim of this chapter is not to assess the claim that activities are necessary constituents of our ontology. Instead I will argue that even if

activities are to be included in our ontology, a commitment to an ontological category of dispositions is required in addition. My argument builds up through the course of this section as I assess whether activities are descriptively fit for purpose, I discuss the criteria of similarity, descriptive accuracy and explanatory unification in turn.

In my discussion of similarity I will hint at a theoretical problem for MDC that may inhibit their ability to capture certain types of similarity statements. I will then show how chemists treat these similarity statements in practice and discuss the role of dispositional properties in a descriptively accurate metaphysics. Both of these discussions point to a need for dispositional properties. I'll then show how commitment to dispositional properties as well as a corresponding commitment to activities improves explanatory unification.

### 3:5:1: Capturing the Similarity Criteria

The aim of my discussion of the similarity criterion is to hint at a potential problem that the entities – activities ontology might succumb to as a result of the absence of a commitment to dispositional properties. I'll begin by discussing the sorts of similarities that are revealed by classifications of chemical reactions as discussed in chapter 2 and that chemists make predictions on the basis of. I discuss the resulting predictive statements and argue that our ontology must contain something modal if it is to be able to ground such statements. I then return to MDC's discussion of activities and suggest that MDC intend a modal reading of activities, however they do not flesh out the metaphysics that underpins this modality. I look at the way modality is accounted for in the related literature and show that these options are not suitable to ground the modal nature of activities. I conclude that activities cannot, as yet, be given a modal reading and additional commitment to dispositions is required to accommodate possibility statements.

Earlier in this chapter I discussed the aims of chemists producing classifications of chemical reactions and their desire to achieve enhanced predictive ability. I showed that classifications are based on structure- activity relations linking

the structures of the reaction centres of molecules with the characteristics of the resultant reaction. Those reactions that appear in the same cluster in the reaction landscape are likely to share other properties in common. This allows chemists to answer practical questions such as these listed by Gasteiger at the start of his investigations in to the classification of organic reactions;

> 'What starting materials and reaction conditions could give a molecule having a desired structure, will the desired reaction actually occur, will the molecule be produced as a major product, will side reactions occur, what is the reaction mechanism, etc.?' (Gasteiger 1997, 210).

On the basis of this discussion we can identify the kind of predictive statements that chemists make on the basis of the similarity relations revealed by the reaction landscape. For example, statement A below which indicates that reactions that fall close to each other on a reaction landscape might be activated by the same catalyst.

A All members of cluster P will exhibit an increase in rate as a result of the presence of catalyst X

Due to the complex chemical environment in which these reactions take place we should not take these statements as necessary. We can imagine a situation in which a catalyst failed to increase the rate of a reaction of one of the reactions in cluster A due to further mitigating factors. For instance the presence of environmental factors that slow down the rate of reaction or the absence of the required conditions for the reaction to take place. As a result we should read the above statement as a possibility statement;

A* It is possible that reactions in cluster P will increase in rate as a result of the presence of catalyst X

Since we already know that at least one reaction from cluster A will increase in rate in the presence of catalyst X we know the possibility statement holds.

We can see an example of this in practice by referring back to the classification of organic reactions discussed in chapter 2.

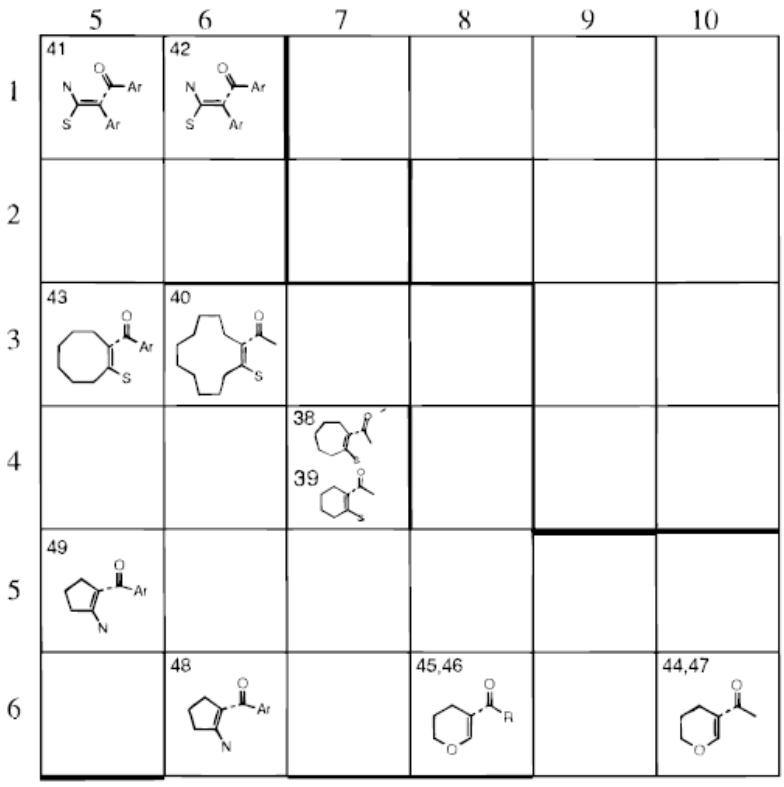


*Figure 18: A cluster of acylations of alkenes from the classification of organic reactions in neural networker (Gasteiger and Chen, 1997, 4037)*

The diagram is a sub section of the reaction landscape containing only the cluster of acylations of alkene reactions. The reactions are labelled with a number and the products of the reactions are inserted into each box with the bond formed during the reaction indicated with a dotted line. We know from prior theoretical knowledge that reaction no.41 is an acylation of a double bond which is doubly catalysed by a sulphur and a nitrogen atom. We also know that reaction 39 is catalysed by a sulphur atom and a carbon atom whilst reaction no 46 is initiated by an oxygen atom although a more activating catalyst is needed (Gasteiger, 1997, 4037). Since these reactions have been grouped together in the cluster, it is suggested that knowledge concerning which entities act as catalysts and under what conditions can be extrapolated from one reaction to another. This leads to the formulation of possibility statements along the lines of; 'it is possible that reactions that are members of the cluster of acylation of alkenes will be initiated by sulphur' (Gasteiger, 2004, 4037). Any metaphysics that is adequate for the classification of

chemical processes in practice must be able to accommodate statements of this form.

### 3:5:2: a Modal Reading of Activities

I've suggested that the classification of chemical reactions in practice involves the formulation of possibility statements regarding how reactions might proceed under a variety of different contexts. In order to accommodate this we need something modal in our ontology. I suggest that MDC have two options. Firstly, they can ground possibility statements by offering a modal reading of activities. Secondly, they can add an extra element to their ontology in order to capture possibility. In this section I will discuss how MDC might proceed with the first of these options. In the next section I will discuss whether a modal reading of activities is feasible. Just as MDC do not explicitly discuss commitment to dispositional properties they also do not discuss in detail the modal status of activities, thus the following section is interpretive.

The first indication that MDC advocate a modal reading of activities is the claim that activities are 'producers of change' (Machamer, Darden and Craver, 2000, 3). In this sense activities are contrasted with entities which engage in those activities and which may exhibit a change as a result of the activity. They add that activities 'are constitutive of the transformations that yield new states of affairs or new products' (Machamer, Darden and Craver, 2000, 4). In claiming that activities *produce change* MDC indicate that activities are causally efficacious in and of themselves.

MDC appear to object to the idea that we should ground interactions between entities in terms of entities and their capacities, and suggest instead that we should treat activities as doing the causal work; 'activities produce changes that constitute the next stage (in the entity)' (Machamer, Darden and Craver, 2000, 5). Again this suggests that MDC treat activities as de re causally powerful with a modal quality. This reading of MDC is backed up by their claim that their treatment of

activities is motivated by ontic concerns (such as their preference for a dualistic substantivalist -process ontology). Thus we can infer the phrase *producers of change* should be read ontically.

In addition, they reject the view that the causal work done by activities in producing such change is brought about via the action of laws of nature. They state 'no philosophical work is done by positing some further thing, a law, that underwrites the productivity of activities' and assert instead that the work of grounding the regularities that exist in nature is done by activities (Machamer, Darden and Craver, 2000, 8). It is stated instead that 'these regularities are non-accidental and support counterfactuals to the extent that they describe activities' (Machamer, Darden and Craver, 2000, 8). Crucially they add that 'counterfactual(s) justifies talking about mechanisms and their activities with some sort of necessity' (Machamer, Darden and Craver, 2000, 8).

MDC do not go on to reveal anything further about this necessity and how it may be cashed out. Part of my project in the forthcoming sections will push MDC further on this point. Thus far I hope to have established the case for reading MDC as committed to activities that are causally efficacious.

### 3:6:3: Accounting for the Modal Nature of Activities

For activities to be modal they must ground notions of possibility and necessity. I will assess strategies for achieving this in the related literature. I will show that these options are not available to MDC and that they must provide a viable alternative account of the modal status of activities or extend ontological commitment to dispositions.

I've already noted that MDC reject the claim that laws of nature exist. Alongside this, MDC are interested in possibility and necessity in the actual world. Their view is compatible with weaker forms of natural necessity so long as they are capable of supporting counterfactuals. For the purpose of my case study, however,

it is possibility rather than necessity that is interesting when evaluating MDC's account and so the following discussion will reflect this.

One option is to look to the powers literature for ideas for how to ground the modality of activities. In particular, I will assess the work of dispositionalists such as Bird and Mumford differ in their approaches but both take necessity and possibility to follow from the causal powers or potencies possessed by individuals.

Since I'm interested in how we ground necessity and possibility in nature; I will put to one side discussions of analytic and logical necessity focusing specifically on de re necessity and possibility. It is helpful to appeal to the work of Mumford who outlines three sources of de re necessity (Mumford, 2004, 166 – 169). The first involves necessary connections between distinct properties so for instance, the property of having shape necessitates the property of having size. The second type of necessary connections are necessary exclusions between properties, for instance, it is not possible for something to have two determinates for any given determinable. (Mumford, 2004, 167).

The third kind of necessity is the necessity that holds between properties that are distinct existences but which are also causally connected. Mumford takes this last form of necessity to be responsible for the dynamic nature of the world since it brings about change in particulars (Mumford, 2004, 168). An example of properties that are linked by this third type of de re necessity (which Mumford calls dispositional necessity) is the property of being fragile and the property of being broken. On Mumford's view this de re dispositional necessity is also metaphysical necessity because the identities of the properties are fixed by the causal powers associated with it. There is no possible world in which something could be that property i.e. be fragile and have different causal powers so that it is not disposed to break when hit (Mumford, 2004, 171).

It is the final kind of de re dispositional necessity and dispositional possibility that I'm interested in as this captures the kind of statements that results from my reaction landscapes. For instance,

A It is possible that reactions in cluster A will increase in rate as a result of the presence of catalyst X

How might MDC be able to ground this kind of metaphysical possibility within their account? My strategy will be to address how possibility is accommodated within the dispositionalist account and use this to spell out what is needed to capture the scientific claims identified above. I'll then address whether activities have what is needed.

Dispositionalists are able to accommodate possibility by appealing to potentiality. Bird is a dispositional essentialist and takes properties to have a causal essence where it is this that determines the property's identity (Bird, 2007, 44). The property's essence is exhausted by the relations it has with other properties such that the property wouldn't be the property it is unless it engages in those relations. Bird characterizes these dispositional properties as potencies. To be potent is to be a potential but also to be real; potencies are actual even when potentialities are not realised, this is in contrast to saying that a property is a potential i.e. not actual. According to Bird;

> 'Part of the being of a potency is the existence of a potentiality. Since potencies are essentially dispositional, every potency will have potential manifestations…We can go further and say that the stimulus – dependent potentiality of a potency exhausts its being. There is no more to the essence of a potency than its potentiality. The combination of a potency's stimulus manifestation are sufficient to identify a potency' (Bird, 2007, 100).

Bird characterises metaphysical necessity and metaphysical possibility by appealing to potencies. Metaphysical necessity is explained in terms of potencies that will always manifest their potentials under the appropriate stimulus conditions. For instance, if it is metaphysically necessary that a body with mass will attract other bodies with mass then;

*all bodies with mass will possess a potency to attract bodies with mass and if there exist other bodies with mass then this potency will always be manifested.*

Bird also explains metaphysical possibility by appealing to potencies that are not yet manifested (Bird, 2007, 100). To take the standard example, when we state that it is metaphysically possible that the vase will break we mean that the vase has the potency fragility and may manifest this potency in response to the stimulus condition. The presence of the non- actualized potency goes some way to providing the non-reductive natural grounding for possibility however Bird further expands on this point by maintaining that there can be no possibility out without a possibility in (Bird, 2007, 105). He states that in addition to unactualised potencies, it must also be possible for the stimulus condition to be activated. In the case of the breaking of the vase if we imagine a situation in which a precious vase was kept in a room which also contained a fast acting deadly chemical such that it wouldn't be possible for anyone to get close enough to strike the vase then it would not be possible for the vase to break (Bird, 2007, 105).

An objection commonly levelled against the dispositionalist is that whilst the account contains potentiality is also is lacking in actuality. It is helpful to raise these objections at this point since I will argue in the next section that in ascribing modality to activities MDC face the opposite problem. In Molnar's 'always packing never traveling' objection it is claimed that an ontology consisting entirely of powers lacks the ontological resources to appropriately characterize the actual world (Molnar, 2003, 174). If the world consists only of powers, then we can give an account of change in terms of the passing around of powers, the breaking of the vase is captured by the passing of powers from the power to be broken to say, the power to cut your hand. The idea is that this leads to a regress since we spell out what is meant by the manifesting of one power by positing another power, which then results in another power and so on. Molner's claim is that there is nothing in the dispostionalist's account that captures the *coming to be* of any of the powers. Armstrong captures Molner's objection as follows:

> 'Given a purely dispositionalist account of properties, particulars would seem to be always re-packing their bags as they change their properties, yet never taking a journey from potency to act. For 'act', on this view, is no more than a different potency' (Armstrong, 1997, 80).

Armstrong sees the need to give some actuality to the world and offers his own account where powers result from the presence of laws acting on categorical properties as discussed in chapter 1. I will discuss this objection to the dispositionalist in more detail in chapter 6 and offer a possible solution however for the moment the discussion provides an interesting perspective on the viability of a modal reading of activities.

I will argue that in contrast to the problems faced by the dispositionalist, MDC have not shown us how to incorporate potentiality into their account of activities. As a result their account lacks the required potentiality to do justice to possibility statement A identified earlier in this chapter.

Consider the statements B and C outlined below. I argue that whether the entities – activities ontology can capture statement B is inconclusive at this point however additional commitment to dispositions is required to ground statement C.

B: It is possible that reaction x will increase in rate in the presence of an increased heat supply

C: It is possible that entity y will engage in a hydrolysis reaction in the presence of water

Statement B is about the reaction itself. MDC appear committed to the view that activities are extended in time. They state that activities have 'temporal order, rate, and duration' (MDC, 2000, 3). This reading of MDC is backed up by Illari and Williamson who state that 'unlike entities, capacities and properties – and other common constituents of ontologies – activities exist only extended in time' (Illari and Williamson, 2013, 5).

If we construe reactions as activities on MDC's view then they must be active and ongoing but also extended in time. I suggest that it is in virtue of being extended in time that reactions may be able to accommodate potentiality. The reaction is ongoing or unfolding in time. It therefore has the potential to change i.e. to get faster if the relevant environmental conditions were to come about. It is intuitive to state

that a reaction increased in rate as a result of an increase in heat energy. It is in virtue of this incomplete or unfinished nature of reactions that the truth of possibility statements may be grounded in them.

MDC do not attempt to give an account of how potentiality arises from activities. The onus is on them to do this if we are to take activities to be modal as they suggest. Nonetheless, at least for this sort of possibility statement that ascribe potentiality to reactions this looks to be a feasible way to proceed. In chapter 6 I will look at the relationship between potentiality and actuality in chemical reactions in much greater depth and use this to formulate a positive proposal for a metaphysics of types of reactions. For the moment it is necessary to comment only that a modal reading of activities may be able to accommodate this kind of example although more work is required to flesh out the details of what this amounts to in practice.

I suggest that the second type of possibility statement is more difficult for MDC to accommodate, consider statements D and E;

D: It is possible that entity X will engage in a hydrolysis reaction in the presence of water

E: It is possible that entity Y will catalyse the hydrolysis reaction

These are both possibility statements formulated on the basis of the similarity relations identified on the reaction landscapes discussed in section 2.4 and therefore need to be accommodated by a metaphysics of classification. The problem is that the potentialities at work in these cases look to be associated with the entities themselves rather than the reactions. As a result I suggest that the potentialities provided by activities will not suffice. We know that activities have spatial temporal locations as well as rate and duration and insofar as they are ongoing they may have the ability to ground potentials. However in the two statements described above the activities in question have not yet come into existence and so cannot ground the potentialities. The hydrolysis reaction has not yet begun. Instead the potentialities are associated with the respective entities.

One response to this is to maintain that the entities have those potentialities in virtue of under lying activities, i.e. the physicochemical variables such as polarity or inductive effect described in the previous section of this chapter. Consider again, the properties used to classify reactions;

1. Difference in partial atomic charges which describes the polarity of the bond

2. Difference in sigma electronegativities which describes the ability of an atom to attract electrons in a sigma bond[13]

3. Difference in pi electronegativities which describes the ability of an atom to attract electrons in a pi bond [14]

4. Effective bond polarizability which describes the tendency of the bond electrons to be distorted by an external electrical field

Each of these properties can be construed as an activity when they are taking place, for instance when an atom is attracting the electrons in a sigma bond. Nonetheless the entity will still possess the potential to engage in a hydrolysis reaction, for instance, even when the lower level activities are not manifesting themselves. This suggests that the potentiality is best construed as a dispositional property had by the relevant entity.

So far in this section I have argued that the entities – activities ontology must have a modal component if it is to ground the possibility statements revealed by the case study. I argued that MDC hint at a modal reading of activities but do not flesh out this account. Secondly, I suggested that even if a modal account of activities could be given for some statements concerning the unfolding of reactions, this potentiality would be unable to capture certain types of possibility statements where the potentiality is associated with the entities themselves. Rather, this potentiality looks

[13] A Sigma bond is the strongest type of covalent bond formed by a head on overlapping of atomic orbitals

[14] A Pi bond is a weaker form of covalent bind due to a reduced overlapping between the atomic orbitals

to take the form of a disposition. I will discuss this claim in detail in the following section.

I will discuss the option in which MDC assert that something that akin to dispositions is included in virtue commitment entities and activities where this does the work of capturing potentiality for them. I will argue that this is misleading. I show that dispositional properties have an important role in scientific practice and are deserving of equal status to entities and activities. To play down their function in favour of a two category ontology of entities and activities violates the criteria of descriptive accuracy and explanatory unification.

### 3:6:4: Descriptive Accuracy

In the last section I argued that the entities – activities ontology is unable to ground certain possibility statements. The aim of this section is to argue that potentiality is an essential ontological apparatus that is required to ground the possibility statements resulting from the classification of reactions in a descriptively accurate manner. I show in practice that potentiality is associated with entities but is treated as distinct from the entity in question and the activity-like phenomena that it is associated with.

In section 3.4.2 and 3.4.3 I discussed two possible characterisations of the property inductive effect firstly as an activity and secondly in terms of dispositions. I will now suggest that a concern for descriptive accuracy means we should prefer a characterisation of physicochemical properties such as inductive effect as dispositional properties. I hinted at my argument in the previous section in which I suggested that potentiality must be contrasted with the actuality associated with activities.

In the section above I listed four properties used in chemical classification of enzymatic reactions as described in case study two in chapter 2. It is the possession of particular determinate values for these properties that ground possibility statements such as;

D It is possible that X will engage in a hydrolysis reaction in the presence of water

The possession of these particular properties makes it possible that X will engage in that particular type of reaction. In the example above if X had difference determinate values for these properties then it might not be possible that it engage in a hydrolysis reaction.

I suggest that a characterisation of these physicochemical variables as activities is misleading and they are better characterized as dispositional properties. The definitions of these properties given in section 3.6.3. suggest that in each case the property described is an ability. This is clear with properties two, three and four. With regards to property one, I suggest that this is also characterised as an ability as the property of polarity is itself characterized as the ability of a molecule to attract an atom or molecule with the opposite charge.

In section 3.2 I described how Illari and Williamson state that we learn about the features of activities through examples. They refer to the following examples 'trigger, binding, phosphorylates, modifying, wrapping, folding, cutting, catalyse, protect, opening, unwinding, supercoiling, breaking, inhibiting, stabilizing' (Illari and Williamson, 2014, 4). However these examples of activities look very different to the properties defined above. These activities are described using verbs whilst the physicochemical variables described above are not active doings but potentials for activities or active doings.

I outlined in the discussion above that MDC take activities are extended in time and can be individuated by their spatiotemporal location, duration and rate (Machamer, Darden and Craver, 2000, 3). These features do not straightforwardly apply to the properties above. The 'ability of an atom to attract electrons' is not extended in time at those times in which it is not manifesting itself however it still exists at this point. It shares the same spatial temporal location as the property that possesses it but it does have an extension in time since it is merely ability. It is the actual attracting of the electrons i.e. the manifestation of the ability that has features

such as extension in time and duration. Chemists use their theoretical knowledge to predict and explain when this ability will be manifested and how strong this ability will be. For instance, an atom with a strong positive charge will possess a greater electron attracting ability.

A further thing to note in favour of this view is that the properties described above are treated as real existents even when their respective activities are not ongoing. A useful analogy concerns the storage of chemical entities when they are not in use. Care must be taken to store chemicals in a safe way, since entities possess the dispositional property 'reactivity' when they are stable, and this property must be treated as real for safety reasons. Similarly *effective bond polarizability* is treated as real when it is not enacted, chemists wanting to manipulate the property to a certain end must be careful to ensure the property isn't stimulated by anything else prior to this.

In addition, the properties described above are treated as independent existents by scientific theories. They can be associated with many different entities and they are given a description within scientific theories that abstracts away from the identity of the entities that they are associated with. This is useful in building up a picture of the way in which the property will behave in different situations. They are also treated as distinct from their manifestations although of course the two are related. This is significant because MDC use a similar argument in order to justify commitment to activities in addition to entities. They state that we can abstract away the entities that take part in that activity to reveal a common structure held by all activities of that type irrespective of the entities that take part in them. MDC use this fact to argue for ontological commitment to activities.

I suggest we should follow chemical practice in distinguishing between having the ability to be perturbed by an electric field and the occurrence of being perturbed by an electric field. The way the definitions of these properties are formulated in chemical practice suggests we should treat these properties as dispositions. The manifestation of the disposition may well be better treated as an activity. I will address this last point in chapter 5 and 6.

One way in which MDC might respond to the problem of grounding possibility is by implicitly committing to dispositional properties via entities. I suggest that this approach would violate the criteria of descriptive accuracy by underplaying the role played by such properties in practice as well as their treatment as distinct existents. Consequently, I conclude that commitment to a separate and explicit category of dispositions is required.

Before going on to discuss scientific understanding it is worth mentioning a point highlighted earlier in chapter 2 concerning descriptive accuracy. I mentioned that the most accurate way to determine the course of a reaction is to give a quantum mechanical description of the reaction mechanism, this would give us a complete understanding of the reaction. However, this is currently beyond our theoretical ability and the best epistemic access we have to the reaction mechanism is via physicochemical properties. I maintain though that even if we were to provide each reaction under investigation with a quantum mechanical description, this would not necessarily best serve the ends of our investigation. Each description would be so fine grained that we would be unable to see the range of similarities that might hold between the different reactions and a new methodology would be required to do this. Perhaps we would return to the identifying similarities on the basis of physicochemical properties of reactions. Consequently, I suggest that on the basis of current scientific knowledge, physicochemical properties provide the best way of grounding objective similarities in nature and should be treated as dispositions.

### 3:5:5: Explanatory Unification

I will now address how the entities – activities ontology fares on the criterion of explanatory unification. It is helpful to refer back to 3.3 in which I characterized the property inductive effect and the hydrolysis reaction in terms of activities and then in terms of dispositional properties. I suggest both options are important for enhancing explanatory unification. Firstly consider the characterisation in terms of activities; this involves the specification of a phenomenon in terms of a lower level mechanism or a bottom out activity. I suggest that characterizing a chemical

phenomenon in terms of a lower level mechanism provides an insight into *how* the activity takes place. MDC state that 'Descriptions of mechanisms render the end stage intelligible by showing how it is produced' (Machamer, Darden & Craver, 2000, 22).

In the case of the chemical reaction between ethane and hydrogen bromide the following reaction mechanism elucidates the various parts of the mechanism thus individuating the entities that undergo the change and the activities that bring it about. With respect to mechanisms, MDC state:

> 'To explain is not merely to re-describe one regularity as a series of several. Rather, explanation involves revealing the productive relation. It is the unwinding, bonding, and breaking that explain protein synthesis; it is the binding, bending, and opening that explain the activity of Na+ channels' (Machamer, Darden & Craver, 2000, 22)

The mechanistic description can then be used to identify other phenomena that are brought about in the same way. As previously mentioned, this is achieved by abstracting away from the individual entities involved to give a specification in terms of types of entities and types of activities. For example a hydrolysis reaction diagram increases our chemical understanding by explaining the various features of the reaction that remain the same irrespective of the entities undergoing hydrolysis. These general specifications then function in scientific theories by giving a unified account of how many instances of that mechanism take place.

I suggest that whilst appealing to mechanisms gives an account of **how** a reaction proceeds, an account in terms of dispositions explains **why** the reactions took place. To give an explanation of what caused each step of this we need to appeal to dispositional properties. To help explore this point I will refer to a possible reaction mechanism between hydrogen bromide and ethene illustrated in figure 19 below.

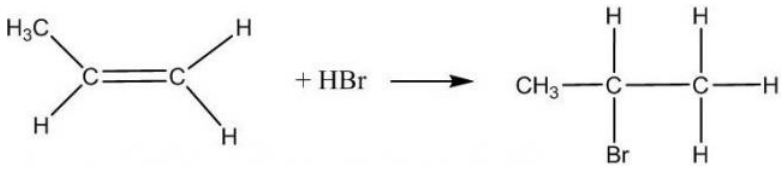


*Figure 19: A reaction between ethene and hydrogen bromide*

The reaction can proceed in one of two ways depending on whether oxygen is present and both these options can be given a mechanistic description. For example, if an oxygen is present then a free radical from an oxygen to oxygen bond reacts with hydrogen from hydrogen bromine molecule to produce a bromine radical. The bromine radical then joins ethene using one of the electrons in the pi bond and this creates a new radical with the single electron on the other carbon atom. This radical reacts with another hydrogen bromine molecule and this creates another bromine radical to continue the process. Eventually the two free radicals hit each other and produce a molecule. The chain then terminates here as no new radicals are formed.

Whilst specifying this mechanism is useful, we can give a different type of explanation which addresses not how but why reaction took place by appealing to the dispositional properties had by the entities involved in the reaction.

1. Oxygen molecules are disposed to be highly reactive due to the extra pair of electrons in the outer shell known as free radicals
2. Bromine is disposed to attract hydrogen in order to share its electron
3. A hydrogen ion is disposed to be highly reactive as a result of having only one electron in its outer shell.
4. A bromine ion is disposed to attract electrons in order to become more stable, it manifests this disposition by reacting with the covalent pi bond
5. Free radical electrons are disposed to be highly reactive due to their having only one electron in their outer shell.

It is these dispositional properties that explain the change in virtue of being producers of the change. This relates to my argument in the previous section in which commitment to dispositional properties is required to accommodate the causal powers had by entities.

Illari and Williamson suggested that activities improve understanding for three reasons; activities are epistemically prior to capacities, activities are conceptually prior to capacities and we can better understand activities by treating

them as distinct beings rather than reducing them to dispositions. My concern for explanatory unification is similar to Illari and Williamson's drive for better scientific understanding, however I am not primarily concerned with debates over whether activities have priority over dispositions or vice versa. Rather, I'm interested in whether activities or dispositions are descriptively fit for purpose with respect to the classification of reactions. Part of being descriptively fit for purpose involves giving explanations that unify many phenomena in such a way that promotes the fruitful development of science. In this respect I suggest that a commitment to dispositions is just as important to providing productive scientific explanations as a commitment to activities. It is physicochemical properties that are crucial to explaining why the reaction proceeded in the way it did and are relevant to meeting the assumption that entities with similar physicochemical variables will engage in similar reactions, on which classification is based.

I suggest that this is a particular instance of a more general relationship between entities, activities and dispositions and that this relationship is essential to the fruitful progression of science via enhancing scientific unification. Dispositions serve the function of anchoring activities to entities. Their function is to trigger a particular activity (in this case a reaction mechanism). This relationship is symmetrical since the end product of a given activity will be entities with certain dispositional properties. If different dispositions anchor processes to entities, then different activities will produce entities with different dispositional properties. Consequently, I suggest that a unified explanation of chemical reactions and their classification requires commitment to dispositions as well as entities and activities. I will return to the relation between entities, dispositions and activities in chapter 6 of my thesis, in which I argue for a three category ontology.

## 3:6:6: Conclusion

In this chapter I have assessed whether the entities – activities ontology proposed by MDC is capable of accommodating the classification of chemical reactions in practice. I was motivated by the appeal to mechanisms in realist accounts

of natural kind classification and the need to address the status of mechanisms as an ontological components for a metaphysics for the classification of reactions.

I began by giving an account of activities as they are outlined by MDC and further developed by Illari and Williamson. I showed that the use of the term activity by MDC is consistent with its use by chemists in QSAR. I've argued that appealing to mechanisms in virtue of the entities – activities ontology is not sufficient to accommodate classificatory practice. I suggested that to meet the criteria of capturing objective similarities the ontology must be able to ground possibility statements and outlined an interpretation of MDC's account on which activities are treated as modal. I discussed how MDC might flesh out the modal nature of activities in practice and concluded that even if activities could ground certain types of potentialities the possibility statements regarding entities and their relation to reactions mean a commitment to dispositions is required in addition to activities. This claim is supported by the appeal to something resembling dispositional properties in chemical practice and the use of dispositional properties in achieving explanatory unification.

In this chapter I have begun the project of addressing which ontological components are required for a metaphysics of classification in practice. I argued that an entities – activities ontology is not sufficient without additional commitment to dispositions. This provides important resources for chapter 6 when I return to the question of which realist approach to kind classification, if any, is appropriate for the classification of reactions in practice. The successful candidate must include a place for dispositional properties. In the next chapter I will examine whether an ontology of entities and dispositions is sufficient without the additional commitment to something resembling MDC's activities.

# *Chapter 4: Can entities and dispositions capture the classification of chemical reactions in practice?*

## 4:1: Introduction

The aim of my thesis is to provide a metaphysics for the classification of chemical reactions in practice. I began in chapter 1 by outlining existing approaches to classification in the current natural kind literature and suggesting these accounts cannot straightforwardly accommodate the classification of non-entity like things. In chapter 2 I assessed two case studies from chemical practice and questioned what a metaphysics of classification must be like if it is to accommodate this practice. I drew out three criteria that a metaphysics must meet if it is to be descriptively fit for purpose. I then related this discussion of practice to the accounts of classification outlined in chapter 1. I suggested that strong essentialist constructivist approaches to classification are not appropriate.

This leaves a variety of weak realist positions which each have the potential to be adapted to accommodate the classification of entities. Each account is committed to different ontological apparatus such as mechanisms, dispositional properties, and processes. In order to adjudicate which account is the most appropriate to classifying reactions I've suggested we need to establish which ontological components are required for a metaphysics of classification.

In chapter 3, I focused on the commitment to mechanisms where this commitment is via the entities - activities ontology. I concluded that if the entities - activities ontology is to accommodate the classification of reactions in practice then it must be adjusted to include an additional ontological category of dispositions.

In this chapter I will address whether the entities - dispositions ontology is sufficient for accommodating the classification of chemical reactions in practice, without for instance, additional commitment to MDC's activities. In section 4.1 I'll examine the difference between the way in which entities and reactions are treated in practice, in section 4.2 I'll examine the difference between the way dispositional properties and reactions are treated in practice. In section 4.3, I'll refer to previous discussion to show that the classification of reactions cannot be accommodated using collections of entities and dispositions in a way that is descriptively fit for purpose. I will conclude that a third category is required to accommodate the classification and will highlight some of the features that this category must have if it is to be compatible with practice. I will call this third category of 'processes'.

## 4:2: Reactions and Entities: a Comparison

My aim in this section is to compare the classification of reactions to the way in which chemists treat entities in practice. By comparing the treatment of entities and reactions I will conclude that for the purposes of a metaphysics of classification in practice, they should be considered as distinct types of ontological entity. I show that there are two key differences between entities and reactions; the first concerns their relation to change and the second concerns the way in which they are extended in time. I will conclude this section with an account of the characteristics of reactions that cannot be accommodated by the category of entities and must be accommodated by dispositions or some combination of entities and dispositions if the entities - dispositions ontology is to be sufficient.

The relation of entities and reactions to change is described by Gasteiger and Engel in their introduction to chemoinformatics. They state that; 'chemistry deals with compounds and their properties and their transformations, thus, two objects have to be considered, compounds and chemical reactions, the static and dynamic aspects of chemistry' (Gasteiger and Engel, 2008, 1).

This indicates that from the perspective of descriptive accuracy, reactions cannot be assimilated into the category of entities but also that they are applicable to different areas of practice. Firstly reactions are the dynamic aspect of chemistry which are responsible for chemical change; 'compounds are transformed into each other by chemical reactions' (Gasteiger and Engel, 2008, 1).

Not all instances of change occur as a result of reactions, for example, mixtures and changes of states involve change but not the making and breaking of bonds. However the notion of reactions as dynamic happenings is a crucial part of chemical practice as reactions are a key means by which entities change.

Entities on the other hand are considered to be static unless they are in a state of undergoing change. Entities can change by gaining or losing properties; for instance a hydrogen atom retains its token identity whilst changing when it gains and loses kinetic energy. Alternatively entities can change by gaining and loosing parts. At the level of atoms or molecules this might happen by gaining or losing electrons. Note, however that at the level of molecular chemistry the properties of molecules that determine identity tend to be microstructural so it is likely that in some cases the gain or loss of electrons would affect token identity.

I suggest that in order to be descriptively accurate our ontology must preserve the relation between the thing that changes and the change itself and thus not assimilate reactions into the category of entities. This is also important if our ontology is to be able to capture the kind of similarities identified in section 3.6.3. Consider, again, the following similarity statements;

B: It is possible that reaction x will increase in rate in the presence of increased heat supply

C: It is possible that y will engage in a hydrolysis reaction in the presence of water

Statement B which concerns a reaction and cannot be reduced to a statement about entities. It is not the entities themselves that are increasing in speed i.e. moving

faster around the container (although this may also occur). Rather, it is the rate at which the entities are transformed from one type to another that increases in rate at higher temperatures. It is important to distinguish these two situations for the purpose of meeting the criteria of explanatory unification. An accurate explanation of why the reaction increased in rate must be an explanation about the reaction itself; such an explanation would accommodate the fact that it is conceivable that the speed of the entities in solution increases but the rate of reaction does not, as a result of other limiting factors. Therefore in order to be descriptively fit for purpose we must treat reactions and entities as distinct.

We can build on this picture of entities and reactions by thinking about how chemical change is enacted. In section 1.2 I made a distinction between an individual reaction mechanism and the reaction as a whole. The reaction mechanism is represented by a reaction diagram and describes how individual atoms react with each other. The reaction mechanism specifies the rearrangement of the atoms and bonds from the reactants to the end product. However, any single reaction will involve many atoms and therefore many individual reaction mechanisms. The exact number of reaction mechanisms will depend on the number of moles of starting products used. The complete collection of reaction mechanisms is referred is known as the reaction. If we look to chemical practice we can see that both reaction mechanisms and reactions are treated as extended in time, each with distinct temporal intervals in a way that chemical entities are not.

Firstly consider the case of enzymatic reaction mechanisms discussed in chapter 2. The resultant classification schemes saw reactions clustered into groups on the basis of similar features; one of these included a similarity in the number of bonds broken during the reaction. In reference to those reactions that broke two bonds in the reaction mechanism the following was said;

> ‘It should be emphasized that two bonds are not necessarily broken simultaneously in these reactions catalyzed by a single enzyme. Either in the breaking of a bond another bond changes its bond order or, after the first bond is broken, a second consecutive step follows (which might be

> spontaneous). However, overall, eventually two bonds are broken or change bond order' (Sacher, Reitz and Gasteiger, 2009, 1529).

This supports the claim that in at least in some cases, a reaction mechanism is extended over time. This concurs with our intuitions about how reactions proceed and indeed our understanding of reaction mechanisms which provides. These reaction mechanisms provide a step by step account of how a reaction proceeds specifying the starting material, the bonds broken, the order in which this occurs, the intermediate material formed and the end product.

The fact that chemists present reaction mechanisms in a step wise fashion gives us further reason to consider them to be non-instantaneous. We refer to the different parts of the reaction mechanisms as occupying different temporal regions; the reaction is never wholly present at any one moment.

In addition to reaction mechanisms, the overall reaction that the individual mechanisms constitutes is also extended in time. We might be inclined to agree with this on the basis of our own empirical experience, such as conducting experiments in chemistry classrooms and measuring the time it took for the reaction to come to completion. Again, this discussion suggests that to be descriptively accurate we must treat reactions as consisting of temporal intervals. The extension of reactions in time can be demonstrated more conclusively by appealing to the field of chemical kinetics; the study of the rates of chemical reactions. I will refer to this discussion of chemical kinetics throughout the rest of this chapter.

The speed at which a chemical reaction proceeds is known as the rate of reaction. We know that there is a wide variety in the rates of chemical reactions from very slow reactions, such as iron rusting, to extremely fast reactions, such as the electron transfer processes involved in biological systems or combustion reactions. When chemists refer to the rate of reactions, more specifically, they are appealing to the rate at which the products are formed from reactants. Therefore to measure a reaction rate, chemists monitor the concentration of one of the reactants or products

as a function of time and the resulting value will have units of concentration per unit time, mol dm-3 s-1.

This definition of the rate of reaction requires one further adaptation to accommodate the stochiometry of the reaction i.e. the number of moles of each reactant and product appearing in the reaction equation. For example, the reaction equation for the well-known Haber process used industrially to produce ammonia, is:

$N_2 + 3H_2 \rightarrow 2NH_3$

where $N_2$ has a stochiometric coefficient of 1, $H_2$ has a coefficient of 3, and $NH_3$ has a coefficient of 2. The rate of this reaction could be determined in any one of three ways, by monitoring the changing concentration of $N_2$, $H_2$, or $NH_3$. However because of the difference in molarity we will get different values for the rate of reaction depending on what we choose to measure. Since the same reaction cannot have two different rates the definition of the rate of reaction is defined as the rate of change of the concentration of a reactant or product divided by its stoichiometric coefficient.

A study of chemical kinetics also reveals some of the factors that increase rate of reaction such as concentration, temperature, pressure and the presence of enzymes. We also know that when all environmental conditions are kept constant the rate of reaction will naturally decrease over time. The reason for this is that each reaction begins with a certain quantity of reactants and in order to undergo a reaction mechanism they must collide with a sufficient amount of energy. Over time more and more of the reactants manage to collide with enough energy and the yield of the reaction increases. As there are fewer and fewer reactants remaining the time taken for successful collisions is longer, meaning the frequency of collisions between those reactants and therefore the rate of reaction slows down. The notion of reactions as extended in time is crucial for capturing the similarities between reactions. For example, reactions clustering together in the reaction landscape will have their rates affected in similar ways by similarities in environmental conditions. They are likely to be affected in the same way by, changes in PH, temperature and

pressure. To capture these kinds of similarity the notion of reactions with temporal intervals is required.

The notion of reactions as extended in time is in sharp contrast to the treatment of entities. I've already highlighted that entities are treated as static existents. We can now add they are treated as wholly present at all times at which that entity exists, this is because an entity does not have temporal parts in the way that reactions do. This can be seen from the specification of entities in terms of static structural descriptions and this is the case regardless of the level of detail utilised by the chemist. The diagram below describes a hierarchical scheme for the representation of a molecule with different amounts of chemical information.

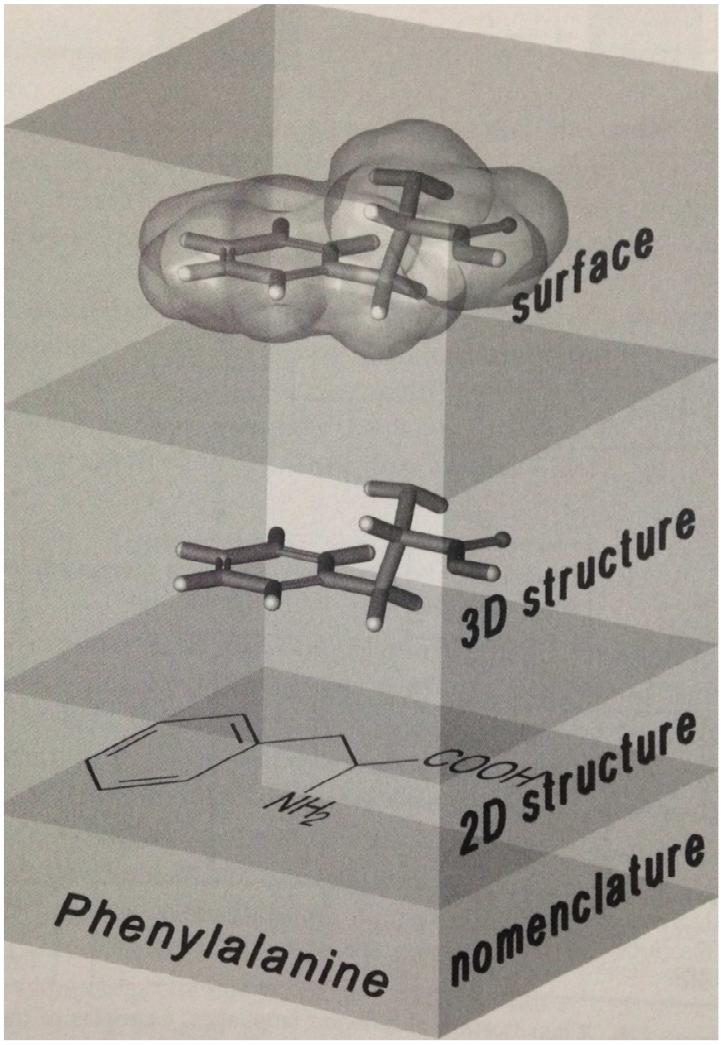


*Figure 20: The structural representations of entities (Gasteiger and Engel, 2008 17)*

The simplest 2D graphical representations are structure diagrams in which atoms are typified by their atomic symbols and the bonding electrons by illustrated lines. Although this is an incomplete and highly simplified representation it allows emphasis to be placed on the most relevant part of the molecule. It's claimed that 'the 2D graphical representation of chemical structures in structure diagrams can be considered the universal 'natural language of chemists' (Gasteiger and Engel, 2008, 170). In chemical practice it is a structural formulation of this kind that describes the token identity of the molecule.

A more complex account of the molecule describes the topology by which atoms are connected specifying the type of bonds and the 3D arrangement of the atoms in the molecule e.g. the positions of the atoms in space, and the angle and

distances between the atoms in the molecule. I discussed this account of chemical entities in section 1.9 and mentioned in particular Hendry's assertion that a 3D specification of this sort was needed to differentiate between isomers of the same compound. Whilst this account gives rise to vague boundaries between kinds it is still a static representation of the compound. The final, most complex, account of entities involves a specification of the electrostatic potential at each point on the entity's surface. These static descriptions of entities concur with the way in which entity classification is discussed in the natural kind literature. The entities involved in classification, whether they be gold, water or tigers, are wholly present at each moment at which they exist. As a result I suggest that the best way to capture the metaphysical picture of the way entities are conceived in practice is on the 3-dimensionalist perspective.

The key tenet of the 3-dimentionalist view is that objects have three spatial dimensions and also endure through time. However the sense in which an object *endures through* time is different to the sense in which it *exists in* the spatial dimensions. According to the 3-dimensionalist when an object exists in time it *wholly exists* at that time. My computer exists wholly in time at time 12:55 just as it did at 12:50. In order to accommodate this the 3-dimensionalist must adopt a notion of identity that is strong enough to allow us to maintain that it is the same computer at 12:50 and 12:55 and weak enough to allow that the computer may have undergone some change. This is in contrast to the way in which my computer exists in space via a collection of spatial parts that each occupies a distinct spatial region (Rea, 2003).

We can then apply this view to my case study. Since objects exist wholly at all the times through which they endure then it follows on the 3-dimensionalist view that objects do not have temporal parts, although of course, there may be spans of time that are associated with different periods at which the object exists. Your childhood, for instance, constitutes a temporal part of your life but this temporal interval is not a part of the object that is you but is a part of your lifespan which runs alongside your you When applied to my chemical case study we can state that

entities are wholly present alongside a temporal interval that constitutes the lifespan of the entity. This is in contrast to the way in which reactions exist in space and time.

One might object to the 3-dimensionalist conception of chemical entities by appealing to Dupré's account of processes. Dupré refers to;

> 'conflict between, on the one hand, life itself as a hierarchy of dynamic and constantly changing processes and, on the other hand, our scientific understanding of living things as grounded on a picture of mechanistic interactions between fixed and statically defined components' (Dupré, 2012, 85).

He attempts to resolve this conflict by arguing that the world is a world of processes and processes have ontological priority. We get the illusion of stable entities when we abstract away from the processes that maintain these entities. He states that 'key concepts in biology…are static abstractions from life processes, and different abstractions provide different perspectives on these processes' (Dupré, 2012, 85).

Dupré might assert that the entities involved in chemical reactions look static but if viewed from a quantum mechanical perspective they are maintained by numerous processes such as chemical bonding. It is these processes that together maintain the stability of the entity by retaining its equilibrium. Dupré raises an interesting question regarding whether commitment to entities is required. I suggest that there is good reason to reject Dupré's objection. I will hint at my response in this section and return to this point in my positive proposal in chapter 6.

My aim is to provide the most appropriate metaphysics for the classification of reactions in practice. In order to meet the criterion of descriptively fit for purpose we need to preserve the relation between change and the thing that is changed. We need to be able to capture the way in which change is brought about where this is something different to stable entities.

In addition, it is particularly important that entities are treated as distinct from the change itself if chemists are to meet the aims of their inquiry. Entities must be treated in the way described above in order to use the similarity relations revealed

by the classification scheme to make predictions, and promote explanatory unification via the fruitful development of science.

Firstly, similarity relations are identified using QSAR and as I described in section 2.3.1. this involves a three stage process. In stage one, a rough classification is used to identify a set of reactions that on the basis of prior theoretical knowledge are known to be similar to each other. Typically, this involves identifying reactions that involve similar entities. The motivation for this step is that reactions involving the same atoms and bonds are more likely to exhibit higher level similarities, such as instantiating the same reactions. Therefore the first stage of classification requires making a distinction between static entities with the potential to undergo a change and reactions as constituting the change itself. The second stage of classification is the application of QSAR prior to the application of neural networking in stage three. The second stage of classification involves an analysis of the properties had by the different entities to determine what sort of changes that particular entity might undergo. Both of these aspects require a commitment to entities as well as dispositions. I will discuss this further in chapter 6.

## 4:3: Reactions and Dispositions: a Comparison

In chapter 2 I argued that at least some of the physicochemical variables used to classify chemical reactions are best characterised as dispositional properties. In this section I will compare chemists' treatment of reactions to their treatment of these physicochemical properties (or dispositional properties). I will use this discussion to show they are sufficiently different to reject the possibility that reactions are appropriately characterised as dispositional properties.

I will begin this section by returning to my discussion of dispositions in chapter 3. I previously argued that the entities – activities ontology is insufficient to capture the classification of chemical reactions on the grounds that activities lacked the required potentiality to make sense of predictive statements and therefore dispositions are needed to fill this theoretical hole. I highlighted a conception of

dispositional properties on which they are thought to be potencies; they are potentials that exist when they are not manifesting themselves. I will focus on potentiality as a defining feature of dispositions.

More specifically dispositions are potentials for something in particular to happen; for example a glass has the potential to break whilst oxygen has the potential to combine with hydrogen etc. With respect to my chemical case study I suggested in section 3.4.3 that dispositions are required to accommodate the following type of statements.

B: It is possible that reaction x will increase in rate in the presence of increased heat supply

C: It is possible that y will engage in a hydrolysis reaction in the presence of water

Both statements are used by chemists to make predictions and tell us what has the potential to happen under certain conditions. Statement C refers to a potential had by one entity whilst statement B predicts how a reaction may change under the influence of certain environmental conditions.

We can begin to compare reactions and dispositions by looking at how reactions are treated in practice. I show that treating a reaction as a potential is an initially intuitive option however I argue that this option neglects half of the story about the nature of reactions.

One option might be to assert that if reactions are dispositions then they must be a potential for something to happen. Therefore just as an entity has a potential to engage in a reaction, similarly a reaction has a potential to bring about a certain end product. This is compatible with statement one above. For instance it seems fairly intuitive to state that the hydrolysis reaction has the potential to bring about the end product Z. We can even explain how this is achieved by giving an approximate specification of the mechanisms by which a hydrolysis reaction operates. The notion of a reaction as a potential for the end product can also be made compatible with

statement two above, if we accept the existence of a causal chain. We can treat the reaction as an intermediate step in the transitive causal chain leading from entities to end products.

There is something intuitively appealing about treating reactions as potentials. Reactions are directed towards a certain end product just as a disposition is a potential for some F to manifest. In addition there is an absence or incompleteness associated with reactions, a reaction may be ongoing but is still incomplete until the appropriate end product has been brought about. This is also the case with dispositions. Reactions and dispositions are also alike in that they bring about their own destruction. The reaction is complete only when it has brought about the appropriate end product. It ceases to occur because the entity ceases to have that potential; it has been actualised.

Nonetheless, there is an opposing intuition which suggests that a reaction is more than a mere potential, but is in fact actual; we might consider a reaction as a *happening* or a *coming to* be. This *coming to be* is not passive in the sense that a glass has the property of being fragile but might not manifest the corresponding manifestation 'breaking'. On the contrary, the reaction is an active directedness towards the potential such that it eventually brings about the destruction of the potential. In other words, the reaction is ongoing. I suggest that a conception of reactions as active and ongoing is crucial if our account is to be descriptively fit for purpose.

This coming to be is akin to the process of unfolding that I discussed earlier in section 4.2 where I described how a reaction is extended in time with distinct temporal intervals. The reaction is not wholly present at any one moment in the way that an object might be, nonetheless a part of the reaction *is present* and *is actual* at any one moment at which it is taking place. This indicates a difference between the sorts of potentials that I discussed in chapter 3 and the notion of a reaction as a potential. The entity waiting in the test tube has the potential to engage in a reaction just as the reaction also has the potential to bring about an end product. However the reaction is also *bringing about* the end product; it is bringing about a change. In

this sense it looks like the reaction is both actual and a potential. It is not clear that the dispositionalist can accommodate this required level of actuality.

This is related to the *always packing, never travelling* objection against the dispositionalist according to which dispositionalism contains too much potentiality and not enough actuality (Molnar, 2003). I previously outlined this objection in section 3.6.3. The claim is the dispositionalist view is problematic because there is nothing that brings actuality to the world. Metaphysically speaking, on this view we can only refer to the passing around of powers that do not instance themselves or pass into actuality since there is nothing in our ontological framework beyond that potentiality. In section 3.5 I argued that the entities – activities ontology does not have access to enough potentiality to capture my case study. I now argue that the lack of actuality on a dispositionalist account of nature is a reason to doubt it can accommodate the classification of reactions. I will return to this point in my positive proposal in chapter 6.

There is also an additional sense in which reactions should be considered as *an active coming to be*. I suggest that we can conceive of interfering with reactions and as a result reactions must be treated as at least partially actual. For example, enzymatic reactions operate under highly specific conditions. The reaction landscape allows chemists to predict such conditions on the basis of their knowledge of similar reactions. An important piece of information is the optimum temperature for enzyme functionality, if the enzyme exceeds this temperature the reaction ceases to occur. This means that we could in practice stop a reaction whilst it was under way, perhaps when only half the expected yield had been produced by altering the temperature. In this case we would not want to say that the reaction had not occurred because it hadn't reached completion, rather we would state that the reaction had partially occurred. I suggest that a descriptively accurate characterisation of reactions involved a recognition that reactions have both potential and occurrent components. In this case the reaction has actively occurs but has the potential to occur further. The relation between the potentiality and actuality is dependent on the unfolding of the reaction.

One might object to this by citing the difference between a reaction and a reaction mechanism. We could stop a reaction half way through and maintain only that some of the reaction mechanisms required for the whole reaction to come to completion had not yet occurred. Perhaps then the potentiality lies in the individual reaction mechanism where these constitute the dispositions and the reaction is a collection of manifesting dispositions?

In the previous section I showed that both the reaction and the reaction mechanism are extended in time; therefore the reaction should also be considered an active unfolding just as the overall reaction is considered in this way. On a much smaller time frame we can conceive of halting an individual reaction mechanism and stating that some of the reaction mechanism had occurred although the potentiality for the end product had not been exhausted.

The intuition that reactions are more than dispositions is also supported by the fact that reactions are measurable and this is a key aspect of chemical practice. Rate diagrams allow chemists to plot the speed at which a reaction is occurring at each point at which the reaction is extended in time.

The concept of a reaction as a change is particularly important here as it is how chemists tend to conceive of reactions. I stated at the start of this chapter that chemists conceive of entities and reactions as two distinct components where by reactions are dynamic and bring about a change in entities. However reactions themselves are capable of undergoing change as well as being the means by which reactions change. I explained in the last section that the rate of reaction tends to decrease over time as molecules are used up in the reaction so the time between collisions becomes longer, thus the reaction slows down. However, there are ways in which this can be negated. If we were to increase the temperature for example the molecules would have more kinetic energy and so the probability of two molecules colliding with enough energy to react will be increased. In addition if we were to increase the pressure of the reaction region then the reactants would occupy a smaller spatial region and so the frequency of collisions would be increased. The rate of reaction can also be altered by manipulating the environmental conditions.

Chemists therefore conceive of reactions as capable of changing and the reaction identity as preserved through this change. This must be accommodated in our metaphysics if we are to capture similarities between how different reactions change under environmental conditions as revealed by the reaction landscape and provide the respective explanation.

I suggest that in order to provide a metaphysical basis for changing chemical reactions we need to treat the reaction as actualising rather than a mere potential. This is because it is unintuitive to state that things that are potentials can also undergo change. Potentials might go in and out of existence but they cannot change in the way that chemical reactions speed up and slow down. Potencies are associated with determinate values, for instance an entity might have a charge of -1 so the determinate value for the disposition is -1. If the entity then becomes more negatively changed and has a change of -3 then we would say that the disposition charge has the determinate value -3. In order to get from a charge of -1 to a charge of -3, it is not the case that the potency itself changes from one value to another, rather the entity itself changes by occupying one distinct value over another. The claim that reactions are dispositions looks to be inconsistent with the claim that reactions undergo change or at least it is unclear how to unify these two propositions. I avoid this problem with my positive proposal on the metaphysics of types of reactions as outlined in chapter 6.

One might object to the idea that reactions change by asserting that this can be captured by the nature of dispositions; for instance by the presence of finks and antidotes. However, this would not be sufficient to accommodate the changing of reactions. Our ability to manipulate and interfere with reactions occurs whilst the reaction is ongoing and actualising itself where the reactions retain their identity through this change.

It’s not clear that it’s possible to characterise the manipulability of reactions using finks and antidotes. Finkish dispositions occur because of a time delay between the occurrence of the stimulus for manifestation and the occurrence of the manifestation and this allows for the object to lose the disposition before the

manifestation has had an opportunity to come about (Bird, 2007, 25). The manipulability associated with finkish dispositions does not convey a change at the level of actuality that would coincide with the reaction getting faster or slower. Rather, the presence of finks represents a failure of particular dispositions to manifest as a result of finks. The same is true in the case of antidotes which occur before the manifestation of a disposition and break the causal chain leading to the manifestation so that if fails to occur (Bird, 2007 27). Again, antidotes cannot capture the manipulability which results in a changing chemical reaction. Antidotes bring about a change at the level of potentiality but this change is not reflected in the actuality of the disposition or reaction. Finks and antidotes, are however still relevant to explaining why certain environmental conditions which are disposed to bring about certain effects, fail to do so but they cannot capture our ability to manipulate reactions when they are in actuality.

## 4:4: Reactions as Collections of Entities and Dispositions

One way to preserve the idea that reactions are dispositions is to reject the premise that reactions change. It could be claimed instead that a single reaction involves the instantiation of many dispositional properties each with different determinate values, in such a way that corresponds to the perceived change. On this view a reaction is associated with multiple entities and their dispositional properties. In this section I will discuss the claim that the metaphysical framework for the classification of reactions can be provided by taking reactions to be collections of entities and dispositions. I will argue that this option should be rejected on the grounds that it violates the criteria of descriptive accuracy, similarity and explanatory unification. I argue that there are important characteristics of reactions that cannot be accommodated on this view due to the problem of arity.

The issue of arity has been discussed by Illari and Williamson (2013) when they describe the properties of MDC's activities. They suggest that entities have a one to many arity such that one entity can attach itself to many dispositional properties. Dispositional properties, on the other hand have a one to one arity

meaning that one token property can only attach to one entity at a time. In their paper *In Defence of Activities (2013)* Illari and Williamson argue that the restricted arity of dispositions leads in some cases to a skewed characterisation of scientific phenomena. They discuss cases such as osmosis and suggest that the phenomenon require many entities and many properties to occur. In addition, an account of the relations between all of these entities and properties is required for a full characterisation of the phenomenon. For example, no single entity has the dispositions 'to osmose' rather the phenomenon occurs as a result of the many interactions between the different entities engaged in the system (Illari and Williamson, 2013, 13). They conclude that we should prefer characterising scientific phenomena using activities rather than dispositions since activities have multiple arity and can attach to many entities and dispositions. In what follows, I argue that reactions also have a multiple arity. They should be treated as a system that cannot be reduced to their constituent parts.

Illari and Williamson also add that there are some phenomena where a characterisation in terms of entities and dispositions is appropriate and the problem of arity does not apply. They state;

> 'This point does not apply equally to all activities, since there are some that are not symmetrical and some that attach quite naturally to a single entity. Consider catalysis – the relation between the catalyst and the reaction catalysed is asymmetric' (Illari and Williamson, 2013, 17).

In the next section I will push the claims by Illari and Williamson further and show that even cases that look to be well accommodated by an ontology of dispositions, such as reaction catalysis, will turn out to be problematic when we study the chemical practice in more detail.

To explore this problem consider again the reaction between ethane and hydrogen bromide to give bromoethane. I will use this reaction to illustrate my point because of its simple and well understood reaction mechanism. The conclusions of this discussion apply equally to the reactions undergoing classification in the case

studies described in chapter 2. The equation for the reaction can be described as follows;

$C_2H_4 + HBr - > C_2H_5Br$

Each reaction mechanism as described above involves multiple entities however the reaction itself involves many instances of the reaction mechanism depending on the number of moles of each reactant that are used. If it is to be successful then the entities -dispositions ontology must be able to account for both of these aspects as both are crucial to practice. An account of the reaction mechanism is important for determining how the reaction will proceed and which end products will be formed. An account of the reaction as a whole or what I refer to as a reaction system is vital for capturing similarities regarding the activation energy or reaction velocity and explaining these phenomena.[15]

It is helpful to begin the discussion with an account of how the reaction mechanism works. Bromoethene is an alkene which means that it contains two carbon atoms held together by a double bond. The double bond is present because both carbon atoms are disposed towards a stable state which is achieved by having a maximum number of electrons in their outer shell. Therefore both carbon atoms are disposed to bond with each other in order to share two sets of electrons. The carbon atoms each bond to a hydrogen atom in virtue of also being disposed towards a more stable state.

In the case of hydrogen bromide, both the hydrogen and bromine also bond covalently due to them being disposed to achieve stability. This results in an unequal sharing of the electrons since bromine has a stronger positive charge and thus is able to exert a greater attractive disposition than the hydrogen. This results in the hydrogen bromide molecule being polar with a partial positive charge on the hydrogen and a partial negative charge on the bromide.

[15] Typically when we refer to a reaction, for example by pointing at a test tube, we are referring to the overall reaction system

The reaction begins with the partially charged hydrogen acting as an electrophile (a substance with a strong attraction to a negative region in another substance). The hydrogen manifests this disposition and takes a pair of electrons from the double bond of the bromoethene leaving a single shared pair of electrons between the carbon atoms and a negatively charged bromine ion. This bromine ion is then attracted to the carbon atom forming bromoethene and the reaction mechanism is complete. I suggest that we are able to characterise the unfolding of this reaction mechanism in terms of entities and dispositions despite their restricted arities, however the situation is more difficult in the case of the whole reaction.

No single entity engages in a reaction; rather a reaction with one mole of reactants will involve $12 \times 10^{23}$ atoms where each of these atoms undergoes a separate reaction mechanism. It is the sum of these reaction mechanisms that constitutes the reaction. In addition, it is the interactions between the entities as the reaction is under way that is crucial in giving a descriptively accurate account of the properties of the overall reaction. The restricted arity of entities and dispositions means such an account is not possible on the entities - dispositions account. I argue this also prevents the entities – dispositions ontology meeting the requirements of, similarity and explanatory unification and as a result it is not descriptively fit for purpose with respect to the classification of chemical reactions.

The assumption behind the investigation into the classification of reactions is that the reactions falling within the same cluster will typically be catalysed by the same enzyme or a closely related protein molecule. Therefore the similarity relations allow chemists to better predict which protein molecules will act as enzymes for which reactions. In addition, similar reactions will have similar reaction properties such as initial velocity, maximum velocity and activation energy and so will proceed in the same way. This allows chemists to predict important features of the reaction related to set up requirements, and yield. It also allows chemists to manipulate the reaction on a large scale, for instance altering the rate as required. These predictions are essential if the classification is to be used for industry applications as discussed in chapter 2.

The problem for the dispositionalist is that the increased predictive power chemists want to achieve by manipulating similarity relation is with respect to properties like initial velocity, maximum velocity and activation energy. However these properties result from characterising the reaction as a whole system involving many reaction mechanisms where the system has a multiple arity.

Consider the property of reaction velocity otherwise known as the rate of reaction. I previously described that the reaction velocity is a measure of the frequency at which molecules randomly collide in the proper orientation and with sufficient energy for the reaction mechanism to begin. Since reaction velocity is a measure of the frequency at which this occurs, it is a property of the reaction and not the reaction mechanism. In addition, I previously described how reaction velocity will tend to slow down through the course of the reaction as fewer molecules are available for collision.

I also described how reaction velocity is dependent on factors including temperature, pressure and concentration. For instance, the more concentrated the hydrogen bromide is within an aqueous solution, the more molecules there are in solution and the more frequently these molecules will randomly collide with each other. In addition the higher the temperature the faster the molecules will move in solution and the more likely they are to collide with sufficient energy for a reaction mechanism to be initiated. Therefore accurate description of reaction velocity that can capture the notion of a collision between molecules requires an account of the relations that hold between the different parts of the system. In other words, reactions, as opposed to reaction mechanisms have multiple arity. Consider for example the Arrhenius equation.

### 4.4.1: Arrhenius Equation

The Arrhenius equation describes the dependence of the rate constant of a chemical reaction on temperature. It is defined as follows;

$$k = A e^{-E_a/(R T)}$$

k = rate constant of reaction

T= absolute temperature in kelvin

E_a = Activation energy

R= universal gas constant with a value of 8.314 J/mol K.

A= pre-exponential factor

k is the rate constant for the reaction being investigated, it is determined empirically for each individual reaction. It is the rate constant that gives an overall indication of how fast the reaction will proceed.

Ea is the threshold energy required in order to for the reaction to begin. A reaction with a large activation energy requires much more energy to be initiated whilst a reaction with a small activation energy doesn't require as much energy to reach the initiated. Typically activation energy is measured in units of kJ/mol.

The pre-exponential factor is a constant that characterises molecular collisions and describes the frequency with which molecules collide in the correct orientation and with enough energy to initiate a reaction. It is determined experimentally as it varies for different reactions. It has units of L $mol^{-1}s^{-1}$ or $M^{-1}s$(for $2^{nd}$ order reactions) and $s^{-1}$ (for $1^{st}$ order reactions).

The first thing to note about the Arrhenius equation is that it implies that chemists treat reactions as distinct unified existences where law like statements hold over the reaction taken as a whole and describe the behaviour of the reaction. In formulating the equation chemists have abstracted away from the entities involved in reactions as well as those properties had by the entities involved and instead characterised the interactions that hold between them. This gives us a general account of the reaction where it is construed as a single system. The reaction landscape reveals similarities in properties such as activation energy and reaction constant which are referred to in the equation and these properties hold over the whole reaction taken as a unified existence. Therefore, in order to capture these

similarities in a descriptively accurate way we must commit to reactions as unified existent rather than as reducible to entities and dispositions.

In addition, an explanation of these properties requires an understanding of the relations holding between the components engaged in the reaction. An account of reactions in terms of collections of entities and dispositions cannot accommodate this due to the restricted arity of dispositions and as a result is not descriptively fit for purpose. As described above it cannot capture the relations between the many collisions which together are responsible for the characteristics of the reaction. The Arrhenius equation promotes explanatory unification by allowing the chemist to read off from it general statements concerning the typical behaviour of any reaction under those conditions. For example, the exponential term in the Arrhenius equation shows that the rate constant of a reaction increases exponentially as activation energy decreases. This means that the rate of a reaction is directly proportional to the activation energy. The rationale behind this is that a reaction with a small activation energy does not require much energy to reach the transition state, and so it should proceed faster than a reaction with a larger activation energy.

The Arrhenius equation also implies that the rate of an uncatalyzed reaction is more affected by temperature than the rate of a catalyzed reaction. This is because the activation energy of an uncatalyzed reaction is greater than the activation energy of the corresponding catalyzed reaction.

The exponential term in the equation involves the activation energy as the numerator and the temperature as the denominator. This indicates the generalisation that a smaller activation energy will have a reduced impact on the rate constant when compared to a larger activation energy. Therefore an uncatalyzed reaction is more affected by temperature changes than a catalyzed reaction.

We are not able to achieve this large scale explanatory unification by reducing entities to collections of entities and their dispositional properties as required by the entities – dispositions ontology. This is because explanations are not relevant to an account of single reaction mechanisms but only to the reaction where the reaction is

construed as a single system made up of many reaction mechanisms. As a result, we must treat each reaction as a single existence in its own right. Therefore I suggest that we must have access to something to something akin to reactions amongst our ontological resources.

One option is to commit to a third ontological category in which reactions fall. This category would be similar in spirit to the activities described in chapter 3, however to avoid the extra ontological baggage associated with MDC's account I shall call this category 'processes'. Whilst reactions would fall in this category, it should also be realistic to expect that the category has the scope to be applicable to other areas of chemical and scientific practice. This option would come at the expense at a minimalist ontology.

A second option would be to address whether it is possible to get access to these processes at no extra ontological cost. In chapter 5, I will examine whether this second option can be achieved by appealing to causal dispositionalism as advanced by Mumford and Anjum. My discussion will focus on whether the causal dispositionalist can ground processes using a distinction between causes and enabling conditions.

Irrespective of whether we get ontological access to processes via a distinct ontological category of processes or via causal dispositionalism the resulting processes must have certain features in line with the discussion in this chapter; they should be modelled on what we know about reactions. An ontological category of processes should be similar in spirt to MDC's activities in the sense that reactions types of changes and the means by which change take place. Typically reactions bring about a change in a relevant entity. However, an ontology of processes must be compatible with the notion that reactions are themselves capable of undergoing change whilst maintaining their identity through this change. Relatedly, reactions are capable of being measured and interfered with.

An account of processes must also accommodate the fact that that reactions are extended in time with temporal intervals and therefore not wholly present at any

one time. We know also that reactions have a multiple arity in order to capture the features of the system that each process constitutes. I will return to this discussion in chapter 6 in which I outline my positive account of processes. I will focus specifically on the relationship between potentiality and actuality in a given reaction system and use this to formulate a definition of a process. In chapter 5 I will examine whether causal dispositionalism can offer a suitable account of processes.

## 4:5: Conclusion

In this chapter my aim was to learn more about the nature of chemical reactions by comparing the treatment of reactions to entities and dispositions in chemical practice. I provided a comparison with the way entities and reactions are treated in practice drawing out key differences between the two aspects of chemical practice. I then compared chemists treatment of reactions with their treatment of physicochemical properties which I've suggested in chapter 2 should be characterised as dispositional.

I argued that reactions cannot be accommodated by taking them to be a collection of entities and their dispositional properties, in a way that is descriptively fit for purpose. A single reaction is more appropriately characterized as a system which cannot be reduced to its constituent parts, i.e. entities and their properties. Rather we need to abstract away from these constituent parts in any one case, substituting them for place holders. We can then examine the more general relations that hold between the place holders in a way that is descriptively fit for purpose, captures similarity relations and promotes explanatory unification. As a result I suggest that we need something akin to reactions in our ontology. One option is to commit to a third ontological category of processes in which reactions fall. Before committing to an additional ontological category of processes I will assess whether we can meet this requirement via causal dispositionalism.

# Chapter 5: Causal Dispositionalism: Getting Processes for Free

## 5:1: Introduction

The aim of my thesis has been to outline the most appropriate metaphysics for the classification of reactions in practice. In chapter 1 I argued that the natural kind literature focuses on the classification of entities and has not addressed in a scientifically informed way the classification of non- entity like things. In chapter 2 I discussed two case studies involving the classification of reactions. I outlined the three criteria that a metaphysics must meet if it is to be descriptively fit for purpose: descriptive accuracy, capture similarity relations and promote explanatory unification. I showed that strong essentialism and constructivism are inconsistent with classification in practice and that a variety of weak realist positions remain viable accounts.

In order to determine which, if any, realist account is most suitable I began to address which ontological components are required in the classification of reactions. In chapter 3 I established that ontological commitment to dispositional properties is required and in chapter 4 I argued that reactions cannot be captured in terms of entities and dispositions and instead a reaction should be treated as a unified, single existent which I have termed a process. We know some of the features that processes must have by appealing to the way reactions are treated in practice.

In this chapter I will assess causal dispositionalism; an ontological framework that if successful offers access to processes at no extra ontological cost in addition to commitment to dispositional properties. As I discussed in chapter 1, if two competing ontologies are able to do the same work then we should prefer the one with the minimal ontological base. Therefore if causal dispositionalism is able to meet the

requirements on being descriptively fit for purpose with respect to my case study and also offers processes in virtue of commitment to dispositions then we should prefer this ontological framework. In this chapter I focus on Mumford and Anjum's account of causal dispositionalism however my conclusions are more general. I consider my discussion to shed doubt on the possibility of getting processes in virtue of commitment to dispositions in a manner that is descriptively fit for purpose.

In section 5.2, I give a general account of causal dispositionalism and in section 5.3, I focus specifically on their distinction between causes and enabling conditions and the relation between the distinction and the dispose towards metaphor. I outline how it might provide the identity conditions for processes. In section 5.4, I discuss whether the distinction between causes and enabling conditions is descriptively fit for purpose. I begin by assessing whether the distinction meets the criteria of descriptive accuracy with respect to the first and second stage of classification outlined in chapter 2. I compare Mumford and Anjum's example of arsenic poisoning to the classification of reactions in my case study. I highlight an important difference between causing an event and causing a process. I conclude that chemical reactions are not individuated on the basis of the dispose towards metaphor. I also focus on the role of perspective when identifying processes. I conclude that Mumford and Anjum cannot meet the criteria of descriptive accuracy.

I then discuss whether causal dispositionalism can capture the similarity relations that hold between reactions. I argue that causal dispositionalism fails this criterion because the dispose towards metaphor is too vague and unconstrained. To meet this criteria Mumford and Anjum must provide a more detailed account of functions which might work in conjunction with claims about powers in order to support explanation and prediction on the basis of similarity relations. Finally I discuss the criteria of explanatory unification. The aim of my case study is a better understanding of reactions for the purpose of improved industrial applications of chemistry. I turn to the way reactions are used in industry and show that the dispose towards metaphor used by Mumford and Anjum does not promote explanatory unification or the fruitful development of science.

## 5:2: Causal Dispositionalism

The causal dispositionalist account advanced by Mumford and Anjum is an application of pandispositionalism to the problem of causation. In *Getting Causes from Powers (2011)* they do not offer a defence of pandispositionalism but accept it as a premise and flesh out the account of causation that follows from it. I have already argued that ontological commitment to dispositional properties is required to accommodate the classification of reactions in practice. Since my aim in this chapter is to assess whether the account of causation can get processes from dispositions I will follow them in assuming pandispositionalism (Mumford & Anjum, 2011, 4). If a pandispositionalist account of causation is able to successfully accommodate scientific practice then this will serve as evidence in favour of pandispositionalism in the context of a broader assessment of the position.

Pandispositionalism is the view that all properties are dispositional. Mumford and Anjum are committed to powers as the fundamental element of their ontology. They identify the 'power to F' with the disposition that has a type of manifestation 'to F,' such that the identity of the power is determined by its manifestation. For instance, we associate the manifestation *dissolving* with the power or disposition *solubility* (Mumford and Anjum, 2011, 6). Properties are taken to be clusters of powers and are had by things. This means that properties are not 'free floating.' For example, the property 'weight' is associated with a cluster of powers including 'the power to make the pointer on the scale move' and 'is had by a packet of sugar' (Mumford & Anjum, 2011, 4). In addition, on the pandispositionalist view, objects possess properties (by virtue of powers) even if the powers in question are never manifested. It is claimed that the property of 'being fluent in German' is had by a person even in the case that the person has the potential power to speak German but refuses (Mumford & Anjum, 2011, 6).

In assuming pandispositionalism the distinction between categorical and dispositional properties is rejected. Mumford and Anjum state;

> 'It is argued by many, however, that at least some properties are non-dispositional or categorical. It is not often said what is meant by categorical, but shape is usually considered a paradigm. A pandispositionalist has to defend the view, therefore that even a property such as sphericity is in reality a cluster of causal powers' (Mumford & Anjum, 2011, 4).

They go on to argue that properties which are traditionally thought of as categorical such as sphericity can be associated with powers such as 'will roll down an inclined plane'. It is on this basis that the property 'sphericity' can be differentiated from the property 'cubic'. Mumford and Anjum rightly note that there will be occasions on which an object possesses the property of being spherical but fails, for instance, to manifest the property 'rolls down a spherical plane,' citing the example of a soap bubble. Nonetheless, their version of causal dispositionalism which uses a vector model of causation is able to accommodate these cases by appealing to interfering factors.

Mumford and Anjum advocate causal primitivism; they take powers to be real existents in the world such that they constitute the most fundamental form of modality. They reject attempts by Ryle (1949), Lewis (1997), and Bird (2007) to reduce powers or dispositions to the conditional analysis (Mumford & Anjum, 2011, 11).

Therefore, according to the causal dispositionalist causation is the passing around of powers. Consider a guitar which is plugged into an amp and then strummed. The guitar has the power to produce a sound wave and thus create an audible noise. This power is then transferred to the amp which in turn has the power to take the sound made by the guitar and produce a louder sound. To summarise 'effects are brought about by powers manifesting themselves' (Mumford & Anjum, 2011, 6-7).

An implication of this view is that it is properties that are the true relata of causation (in virtue of the powers from which they are constituted). In everyday life we tend to think about causation in terms of events or facts, for instance, the event of the 'earthquake' caused the 'breaking of the vase' or the fact that 'the earthquake

occurred' caused the fact that 'the vase is broken'. Nonetheless, it is asserted that both of these accounts of causation are true in virtue of properties doing the causal work. As Mumford and Anjum state 'objects, facts and events can all be involved in causation, on our view. But they are involved because of the powerful properties that they contain' (Mumford & Anjum, 2011, 2). When Mumford and Anjum state that 'smoking disposes cancer' this statement is true in virtue of the possession of the relevant powers. For example, the smoking of a cigarette involves the manifestation of powers that dispose towards cancer. In the same way chocolate only disposes towards happiness in virtue of possessing a power that disposes towards happiness.

A controversial aspect of their account which I will refer to throughout this chapter is that powers are taken to have a direction and an intensity. This allows for a vector analysis of causation which is used to provide an insight into the passing around of powers. For instance, since the smoking of a cigarette has the power to cause cancer, it disposes in the direction of cancer, and it does this with a greater intensity than, perhaps, living close to a mobile phone mast. The question of whether the presence of this power is essential to what it is to be chocolate is not discussed. Mumford and Anjum recommend representing powers in diagrammatic form as shown below:

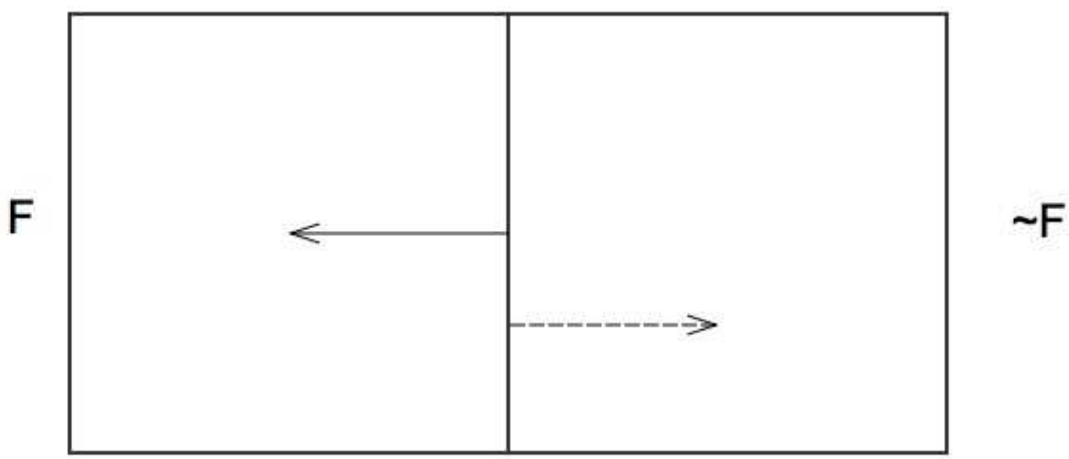


*Figure 21: a vector diagram showing the power of smoking to cause cancer where F is cancer*

The power of smoking to dispose towards cancer can be contrasted with exercise which disposes away from cancer and is represented by the dotted arrow above. Vector diagrams are used to flesh out the various causal factors at work in producing a given effect. In this respect Mumford and Anjum evoke Mill's notion of total cause and reject Lewis's counterfactual dependence account of causation. They aim to do justice to the fact that causation is complex and achieved only as a result of numerous factors working together. They see each cause or power as making a contribution to bringing about the effect and therefore all causes are ontologically on a par. Their commitment to the total cause of an effect is a central tenant of their causal dispositionalism. Mumford and Anjum also make the controversial decision to exclude negative causes and causes by absence, on the grounds that they are not ontologically real. Since this is not relevant to my argument, for the purposes of this chapter I will grant them this assumption.

The notion of total cause and the vector analysis is conceptualised using the threshold model of causation, whereby the threshold represents the minimum combination of powers required to bring about the effect. This is an extension of the notion of mutual manifestation partners. Consider the causal factors that contribute towards the burning of a fire (represented as G on the vector diagram). These include the presence of oxygen, the striking of a match, dryness etc. If a sufficient number of these powers are present they will combine in the vector space and the threshold condition will be overcome. The threshold condition is indicated by the vertical dashed line.

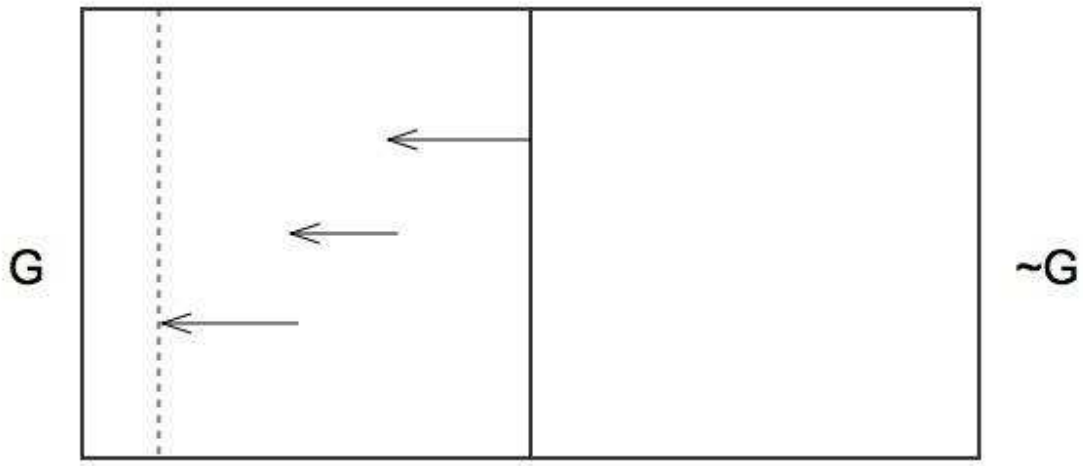


*Figure 22: Vector analysis representing the addition of powers to bring about the effect G*

The examples cited above model the relationship between the compositional and resultant power on the principle of additive composition. The effect is the sum of the constituent powers however addition is only one way in which powers operate. Mumford and Anjum advocate compositional pluralism, whereby there are numerous potential functions that govern how powers combine (Mumford and Anjum, 2012, 96 – 101).

One example of non- linear combination is gravitational attraction where mass and distance combine to produce a resultant force the size of which is governed by the inverse square law. Mumford and Anjum also refer to overdose cases in which adding additional amounts of the same power does not produce an increasing tendency to the same effect. For example, a drug will tend to have an increasingly positive effect on health up until the optimum dosage level, after which it will tend to have a negative effect on health as a result of overdose (Mumford & Anjum, 2011, 96).

In other cases two powers acting in isolation from each other will dispose towards an effect F, however when acting together will dispose away from F. The most common examples of this kind of antipathetic case arise in medicine. Mumford and Anjum discuss the case of Clonidine and Beta-blockers which both individually

dispose towards low blood pressure but when taken together have the opposite effect (Mumford and Anjum, 2011, 91). They conclude that there are different functions that govern how powers combine, but that we should not treat such functions as laws of nature. I shall return to the question of functions in section 5.4.3.

It is worth noting that, non-linear addition of powers has important implications for the debate surrounding emergentism;

> 'Many natural phenomena involve interaction of the components where they produce something together that is not the mere addition of the components. This involves a genuine joint effort of two or more powers where the resultant is composed by some non-linear function. Any such function could be involved: multiplicative, inverse square, or far more complex' (Mumford & Anjum, 2011, 98).

The coming together of powers to do joint work may produce an effect that bears no resemblance to any of the component powers; the effect is more than the sum of the parts. In this sense compositional pluralism introduces an element of emergentism although this is described as 'weak, uncontroversial emergentism' in which a supervenience relation holds. The presence of identical component powers will result in the same resultant power. Nonetheless this isn't to suggest that the same outcome would occur, merely that the resultant power would dispose towards it. (Mumford & Anjum, 2011, 100).

The various objections I will raise to the causal dispositionalist account focus on the notion of 'disposing towards' and the work this does for their account. Mumford and Anjum do not flesh out what it is for one thing to dispose towards another but illustrate by examples. I argue that this is insufficient to establish their account. With regard to the above discussion of the functions that govern how powers combine with each other I argue that a more nuanced account of the place of functions within their ontology and their relationship to powers is required if causal dispositionalism is to accommodate scientific practice.

In chapter 2 I outlined the constraints on my project and in order to accurately assess the causal dispositionalist project I need to understand the constraints that

their account of causation is working within. Firstly with respect to the scope of the project they claim that causation in physics has received the majority of attention in the literature and that there is reason to believe that this is unwarranted. Causation occurs not just in physics but in biology, psychology, economics and society generally and it is important that we are able to give an account of these cases. In so far as reductionism to physics remains only a possibility we should be able to provide causal explanations at the most appropriate level (Mumford and Anjum, 2011, 101). A causal explanation of why I crossed the road is perhaps best provided in terms of my fear of dogs rather than the firing of neurons although this may provide a true description of the situation.

Secondly, with respect to the relationship between metaphysics and empirical science Mumford and Anjum suggest that the two disciplines should interact through a reflective equilibrium. A metaphysics is strengthened by an understanding of the empirical science and empirical science can also benefit from reflecting on the metaphysical assumptions that underlie it. They state that 'our philosophical theory should thus both inform and be informed by our concrete understanding of causation. Our knowledge of causation is best developed by understanding both in tandem, but where neither comes first' (Mumford & Anjum, 2011, 215).

Consequently, if causal dispositionalism is to be philosophically respectable then it must be compatible with contemporary scientific practice. Mumford and Anjum go to some lengths in *Getting Causes from Powers*, to show that their account can accommodate biological practice, it is my aim in this chapter to assess whether their account can accommodate the classification of chemical processes in practice. I will argue that causal dispositionalism cannot do so in a way that is descriptively fit for purpose.

## 5:3: Enabling Conditions and Causes

In section 5.2 I provided an exposition of the pandispositionalist account of causation. In this section, I will focus in on the role played by causal processes and the ontological distinction that is drawn between causes and enabling conditions. I will provide a brief description of this distinction and the motivation for its introduction. An account of these motivations and the work that the distinction does in each case will be important to my analysis in section 5.4 of whether the account can meet my criteria. The distinction between causes and enabling conditions can be summarised as follows;

*Causes will dispose towards an effect whilst enabling conditions do not dispose towards or away from an effect.*

Mumford and Anjum add that;

> 'We can have cases where a caused b and b caused c but it is not the case that a caused c. The reason for this is that while a disposed towards b, and b in turn disposed towards c, there was nevertheless no disposition from a towards c' (Mumford and Anjum, 2011, 176).

In this case a enables c but does not cause c. It is a mere enabling condition for c. At times Mumford and Anjum refer to enabling conditions as *sin qua non*, for instance they state;

> 'Your grandfather's conception is certainly a necessary condition for you scratching your nose, in the sine qua non sense. You wouldn't have scratched your nose without it. But it is not a cause because it didn't dispose towards it' (Mumford and Anjum, 2011, 176)

Enabling conditions or sine qua non conditions are at other times referred to as causally irrelevant;

> 'The vector model enables us to separate causally relevant from causally irrelevant powers, as the first would dispose with some intensity within the model's quality space while the latter would not dispose in either direction' (Mumford & Anjum, 2011, 26).

As I mentioned earlier in this chapter, a key motivation for the introduction of the distinction between causes and enabling conditions is Mumford and Anjum's desire to retain the idea of the total cause of an effect. Mumford and Anjum accept Mill's thesis that all causes of an effect are ontologically on a par. They refer to the straw that broke the camel's back analogy and argue that even though different powers might contribute in different amount they are all equally significant in bringing about the effect. As a result they reject the distinction between causes and background conditions;

> 'the grounds for asserting the distinction [between causes and background conditions], however, seem entirely pragmatic: usually to do with explanatory practices and assumptions rather than to do with the efficacious powers in the world. The distinction is therefore primarily an epistemic one, rather than a matter for the ontology of causation' (Mumford and Anjum, 2011, 32).

The reasoning behind the rejection of the distinction between causes and background conditions will be important to section 5.5.3 as I will suggest that their own distinction between causes and enabling conditions suffers from a similar problem.

In addition, whilst they embrace the notion of the total cause they also acknowledge an objection to it and the need to pose some limit to the transitivity of causation in order to support their thesis that cause and effect are simultaneous. They state; 'there may be an objection that Mill's notion of cause includes too much. Might every previous event in the universe count as a cause of every later effect, or at least everything in an event's backwards light cone?' (Mumford and Anjum, 2011, 13).

To be forced to admit that everything in an event's past acts as a cause is both counterintuitive and seems to devalue the notion of cause. Consequently Mumford and Anjum look for a way to restrict what should fall within the notion of the total cause for a given effect. The distinction between causes and enabling condition is an attempt to help them achieve this aim. It is worth quoting them in full on this point as I shall return to it later in the chapter.

> 'Causal dispositionalism, however, has some resources for limiting the causes of an effect... We count only as a cause of an effect something that disposes towards it and not everything in the backwards light cone will have done this. If you speed up your walking, for instance, there will be many factors in the past that simply did not bear on it: they had no disposition to increase or slow down your walking. Causes can be big, therefore, as Mill's notion suggests, without being too big' (Mumford & Anjum, 2011, 13).

Modifying Mill's concept of total cause by introducing the distinction between enabling conditions and causes allows for all causes that contribute to the overcoming of the threshold condition to be considered ontologically on a par. It also provides principled justification for limiting the remit of the total cause. We can see the distinction in action via two case studies provided by Mumford and Anjum.

Firstly they describe the process by which arsenic causes death when ingested. They argue that we can attribute this power to arsenic since it initiates a causal chain which begins with the disruption of ATP production leading to organ failure and then to death whereby *each stage of the process disposes towards the next*. As a result the causal chain is transitive and it is correct to assert that arsenic causes death.

Secondly they describe a causal chain that begins with weather conditions in the Caribbean and ends with a broken elbow but where causation is not transitive as a result of an enabling condition in the causal chain.

> 'Conducive weather in the Caribbean leads to a bumper banana crop. The fine crop leads to reduced prices and this influences you to buy bananas. Having bought the bananas, you eat them more often and on one such instance you discard the skin. Later, you slip on the skin, fracturing your elbow. Did the good Caribbean weather cause you to fracture your elbow?' (Mumford & Anjum, 2011, 171)

From this, the following causal chain can be identified;

Hot weather → More bananas → Cheaper bananas → I buy more bananas → I eat bananas more often → I slip on banana skin → I fracture my elbow

Mumford and Anjum's point is that causation is not transitive because there is

nothing about the hot weather that disposes towards my fractured elbow. Although they do not point it out themselves it seems that the point at which transitivity breaks down and thus the existence of the enabling condition must occur between eating bananas more often and slipping on the banana skin.

To summarise Mumford and Anjum have rejected the distinction between background conditions and causes on the basis that identifying a special or more significant causal factor involves an appeal to pragmatics and this shouldn't be tolerated in questions of ontology. Instead they embrace the idea of a total cause where all the powers that contribute towards an effect are ontologically on a par. They then seek to limit the total cause via the presence of enabling conditions in the causal chain that do not dispose towards the end effect and therefore limit transitivity.

It is important to make clear the direction of explanation at work. Failures in transitivity result from the presence of enabling conditions in the causal chain and the distinction between enabling conditions and causes rests on the notion of disposing towards. The distinction between causes and enabling conditions therefore provide the identity conditions for causal processes such as the one by which arsenic disposes towards death as described above. In what follows I will assess whether the dispose towards metaphor is capable of bearing this weight.

A further motivation for Mumford and Anjum's introduction of the distinction is their belief that cause and effect are simultaneous and non-instantaneous. They object to ascribing temporal priority to causes over effects on the grounds that this leads to a regress. If causes are prior to effects then something must be said about the temporal gap between them and in particular what causes the gap to close and the effect to come about.

By appealing to an ontology of powers the causal dispositionalist has the resources for overcoming this problem. Since metaphysically speaking properties do the work of causation not events they argue that it is mistaken to assume that cause precedes effect on the grounds that one event precedes another. They describe the

dropping of sugar in tea and suggest that dissolution is a causal process in which cause and effect are simultaneous. For instance, we can imagine stopping the process half way through and exclaiming that half the sugar has dissolved. We wouldn't want to wait to the end of the process to say the effect occurred. Instead it is claimed that the 'the cause will be depicted as merging into and becoming the effect through a natural process' (Mumford and Anjum, 2011, 107).

They use the distinction between enabling conditions and causes to reject any claim that one process causes another and therefore to rebut any objection to the simultanity of causation; the idea is one process merely enables another. I will not deal explictly with the claim that cause and effect are simultaneus but will discuss the treatment of processes that is required to establish this claim. I will argue that it is not descriptively fit for purpose with respect to my case study.

## 5:4: Causal Dispositionalism: Descriptively Fit for Purpose?

In the above section I have outlined Mumford and Anjum's causal dispositionalist account. I focused specifically on Mumford and Anjum's distinction between causes and enabling conditions and the work that the distinction does for their account. I also described how the distinction rests on the disposing towards metaphor. In the remaining part of this chapter I will discuss whether this distinction is descriptively fit for purpose with respect to my case study. If it is successful and Mumford and Anjum's causal dispositionalism is able to provide the identity conditions for processes then their account could give us the processes we required as discussed in chapter 4 at no extra ontological cost. I will begin by looking at the criteria of descriptive accuracy and then turn my attention to similarity and explanatory unification.

### 5:4:1: Descriptive Accuracy

In this section I will argue that the distinction between enabling conditions and causes does not accurately capture the way in which reactions are individuated

in practice. I will discuss this point with respect to the second stage of the classification process and then with respect to the first stage of classification.[16]

#### 5.4.1.1: Stage Two of the Classification Process

In this section I will proceed by clarifying how Mumford and Anjum use the distinction between enabling conditions and causes to individuate processes and then I will compare this to the treatment of reactions in the second stage of classification in my case study.

In their discussion of the biological process associated with 'arsenic causing death', Mumford and Anjum state;

> 'Arsenic, can be thought of as having multiple powers: of disrupting ATP production, of causing organ failure, of killing. A reason why we can attribute all these powers to arsenic is that it is able to initiate a biological process, going through various stages' (Anjum & Mumford, 2011, 168).

They claim that this constitutes one biological process because each step in the causal process from ingestion to death disposes towards the next and therefore the causal chain is transitive. We can identify the process as follows;

Ingesting arsenic → Disrupted ATP production → Organ failure → Death

The process by which arsenic leads to death is an example of what Mumford and Anjum refer to as a 'biological process' (Mumford and Anjum, 2011, 168). They individuate the process from its context in virtue of the enabling conditions versus cause distinction. Other factors that form part of the causal chain that leads to 'death' do not form part of this biological process because they are merely enabling conditions rather than causes and so their presence produces a break in transitivity.

I argue that the disposing towards metaphor can be made applicable to the second stage of classification of reactions however it does not give identity

[16] I discuss the two stages in this order since it is the second stage of classification that is the more central component of my case study.

conditions for the reactions in my case study as is suggested in the case of arsenic. I argue that the reason for this involves an important difference on the causal dispositionalist account between the causing of an event and the causing of a process.

It is worth mentioning that Mumford and Anjum themselves hint at this difference although they do not explore it in detail. As I outlined in section 5.2 Mumford and Anjum discuss the threshold model of causation and conclude that x causes event y if and only if x disposes towards event y. This is the case regardless of whether x is sufficient for bringing about the event y. This account allows Mumford and Anjum to maintain, for example, that the presence of oxygen disposes towards the fire and is therefore a cause of the fire.

However, in their discussion of processes Mumford and Anjum hint at a different account. They state;

> 'According to the causal dispositionalist theory, the cause of each process is the various mutual manifestation powers that, having come together, do their joint work and go through a transformation: a change of properties…As causation typically involves changes, it thereby makes new powers available for composition and thus instigation of new causal processes. But it would be wrong to think of this as one process causing another in a sequential temporally separated chain. All it does is contribute a power or powers to a further process that might occur if the other partners for that process also become available' (Mumford & Anjum, 2011, 126).

With respect to processes, Mumford and Anjum seem to maintain that contributing a power is not enough to be considered part of the cause of a process. This suggests something else is required, however they do not specify what this extra requirement amounts to. Nonetheless a consideration of the difference between causing processes and causing events sheds light on how the dispose towards metaphor applies to my case study.

Consider again, the case of the burning of the house. We can list the factors that dispose towards the burning of the house such as the presence of oxygen, the presence of fuel and the striking of the match. As Mumford and Anjum rightly point

out each of these factors forms part of a causal chain that leads to fire. Nonetheless I suggest that by identifying these factors Mumford and Anjum have not individuated the specific transitive causal process by which the house is burnt down. They have successfully identified factors that form part of the causal chain that leads to the burning of the house but they have not given identity conditions for the process. There is an important difference between this case and the case of arsenic described above in which Mumford and Anjum claimed to have isolated a section of the causal chain that is individuated by the presence of enabling conditions and labelled it a biological process.

This point can be made more obvious with a consideration of my case study. Consider again the classification of reactions on the basis of six physicochemical variables. I argued in section 3.5 that these physicochemical variables should be characterised as dispositional properties. I also described in section 2.2 how each reaction is associated with values for each of the six properties and these six values are thought to encode the reaction. This encoding of reactions is taken to be sufficiently reliable to retrieve accurate similarity relations between the different reactions. At first glance there is a sense in which causal dispositionalism does capture my case study. The belief underlying QSAR is described as follows;

> QSAR: the reaction centres of entities that possess similar physicochemical variables will undergo similar kinds of reactions

An equivalent statement can be made for causal dispositionalism;

> Causal dispositionalism: entities with similar powers operating under similar functions will undergo similar reactions.

The six determinate properties could be construed as vectors that each dispose by varying amounts to the instantiation of a particular reaction.

It is useful here to return to my discussion in chapter 4.5. I argued that reactions are processes but the processes are defined in terms of their end products. For instance, a hydrolysis reaction is defined as the breaking of a bond due to the

presence of the polar change on a $H_2O$ molecule. This definition was used to isolate this particular group of reactions that are similar enough to undergo QSAR analysis.

I suggest this helps illuminate how the dispose towards metaphor applies to my case. In so far as the physicochemical variables encode hydrolysis reactions, they dispose towards the pre-specified end product occurring. They are a strong indicator that this reaction will occur.

As a result, I argue that the identification of these six properties does not provide the identity conditions for the reaction process by individuating the state and end points of the process. Rather by identifying these properties chemists have highlighted parts of the causal chain that dispose particularly strongly towards the end product associated with the process. There is a clear difference in the way in which reactions are individuated and the case of the 'biological process' involving arsenic.

As I discussed in section 2.1 a full account of the causal process (or what chemists refer to as the chemical mechanism) by which a reaction comes about requires a quantum mechanical specification of the reaction mechanism including reference to the characteristics and movements of the atoms and bonds. I explained that such an account is currently beyond the capabilities of chemistry and physicochemical variables are used instead since they are thought to be the best indicators of similarities in reactions mechanism which are beyond our epistemic reach. As a result I suggest that causal dispositionalism fails the criteria of descriptive accuracy with respect to stage two of the classification process. In practice reactions are not individuated using the dispose towards metaphor or the distinction between enabling conditions and causes which is built on the basis of this metaphor.

#### 5.4.1.2: Stage One of the Classification Process

It is also worth assessing the descriptive accuracy of the causal dispositionalist account against stage one of the classification process. This highlights another respect in which the causal dispositionalist account fails to meet the criteria of

descriptive accuracy whilst revealing an aspect of chemical practice that will be relevant to my positive proposal outlined in chapter 6. My discussion also hints at a tension within the causal dispositionalist account.

I will focus on the role of perspectivalism when identifying reactions. Mumford and Anjum indicate the question of the intensity and direction of powers is an empirical matter;

> 'Substances can be more or less explosive, flammable, corrosive, volatile, soluble, poisonous, alkaline or acid. Some of these intensities are already quantified by a standard scale, such as using the pH scale for acid and alkaline. The understanding of their intensities is regimented in a robust scientific theory. Some may be less regimented. There may not be an exact science that measures degree of fragility. But clearly this is an empirical matter: there could be one' (Mumford and Anjum, 2011, 25).

Appealing to scientific practice when examining the presence of powers is a sensible approach; the best evidence concerning the properties that are had by entities, and the direction and intensity of powers comes from science. I'll follow this approach in the following discussion.

Chemists are interested in solving particular chemical problems and this directs their inquiry. In case study two chemists were interested in improving the efficiency of hydrolysis reactions. Therefore hydrolysis reactions were identified as the activity of interest with respect to QSAR and token instances were identified on the basis of a theoretically prior definition of the reactions. Hydrolysis reactions are defined in terms of a specific start and end point as previously discussed. Given the interest directedness of the inquiry we can conceive of a different situation in which another reaction or process was investigated and so another end point is specified but where this new type of process involves a hydrolysis reaction as a component part.

To explore this point consider again the hydrolysis reactions discussed in chapter 2. Organic chemists interested in the making and breaking of bonds will take the process to end when a hydrolysis reaction has taken place, that is, when water

has been added to the original molecule such that both the molecule and the water split in half forming a hydroxide and with the remaining components combining with the positive ion. They will consider this to be one distinct process. Note that on Mumford and Anjum's view this reaction process ends due to the presence of an enabling condition; the formation of the end products of the hydrolysis reaction do not dispose towards the next part of the causal chain. I suggest this claim is problematic since the end products of the process have multiple powers that will dispose towards in lots of different directions. I maintain that whether we choose to take them to be part of the original process depends on the particular interests of scientists.

Consider one situation in which hydrolysis reactions occur inside the body. During the process inside the body in which *proteins are prepared for their role in digestion*, a hydrolysis of proteins occurs producing amino acids. However these amino acids then react with glucagon which is a catabolic hormone that mobilizes amino acids into blood. The amino acids then undergo polymerization to produce more useful proteins. The chain can be described as follows;

Water reacts with a peptide bond on a protein → the protein splits into smaller chains of amino acids → the amino acids react with glucagon → the amino acids enter the blood stream → the amino acids undergo polymerisation to form new proteins

The process by which proteins are prepared for their role in digestion involves hydrolysis but the end products of this hydrolysis then dispose towards a reaction with glucagon and form part of a much bigger biological process. Hydrolysis occurs in lots of different biological and chemical contexts and in each case it might reasonably be thought to contribute powers that dispose towards the next stage of that particular chemical or biological causal chain.

I suggest that the identity conditions for what chemists might refer to as biological or chemical processes in stage one of the classificatory process are determined by the broader context of the scientist's work and in particular what they want to explain. For the causal dispositionalist this means that whether something is

considered to dispose towards the next stage of the process i.e. whether it constitutes a cause or an enabling conditions, is also dependent on the aims and interests of the scientists.

The problem for Mumford and Anjum is that the impact of interest dependence on the transitivity of causation is not consistent with the rest of their account. I suggest that the role of contextualism and pragmatics goes much deeper into the causal dispositionalist account than can be consistent with their initial position and as a result their account is brought into tension. Consider again the reason why the distinction between causes and background conditions was rejected. Mumford and Anjum state;

> 'the grounds for asserting the distinction [between causes and background conditions], however, seem, seem entirely pragmatic: usually to do with explanatory practices and assumptions rather than to do with the efficacious powers in the world. The distinction is therefore primarily an epistemic one, rather than a matter for the ontology of causation' (Mumford and Anjum, 2011, 32).

The causal dispositionalist wants to treat all causes as ontologically on a par. They suggest to prioritize certain causes over others rather than cite the 'total cause' of an effect would require us to appeal to epistemic considerations and this is an illegitimate move when investigating the metaphysics of causation. I challenge whether Mumford and Anjum are able to remain faithful to this view given the above discussion.

Since the specification of processes in practice involves an appeal to pragmatics they are unable to get an account of a natural process that meets their needs or is compatible with my case study. The distinction between causes and background conditions was rejected because it left room for user 'pragmatics' and according to Mumford and Anjum dissolved into an epistemic distinction. I suggest that the distinction between causes and enabling conditions fares no better. If they are to reject the distinction between causes and background conditions and replace it with a new distinction between causes and enabling conditions, then the latter

distinction should not suffer from the same problem for which they rejected the former.

There is no real, ontological distinction between enabling conditions and causes, it is a tool that helps us isolate a process that is undergoing a particular empirical inquiry in a given domain. The classification of reactions in chemistry is conducted on the basis of pragmatic interests. I shall return to this point in chapter 6. As a result I suggest that causal dispositionalism cannot give an account of processes that meets my criteria of descriptive accuracy.

### 5:5:2: Similarity and Explanatory Unification

In this section I will address whether the causal dispositionalist account can capture the criteria of similarity and explanatory unification with respect to my case study. I will argue that causal dispositionalism fails both criteria as a result of the vague and unconstrained notion of the disposing towards metaphor. It is for this reason that I will discuss the two criteria side by side. I begin by assessing the causal dispositionalist's ability to capture the similarities revealed by the reaction landscape and will go on to discuss its ability to explain the industrial applications of enzymatic reactions in a way that promotes explanatory unification and the fruitful development of science.

The vague nature of the dispose towards metaphor can initially be illustrated through examples. Consider the enzymatic reaction described in chapter 2 between ethyl ethanoate and dilute hydrochloric acid. The ethyl ethanoate reacts with water and acid acts as a catalyst. Chemists have provided a rough characterisation of how the underlying reaction mechanism proceeds. For present purposes I'm interested only in the first stage of the reaction mechanism. Ethyl ethonate is a stable compound held together by covalent bonding;

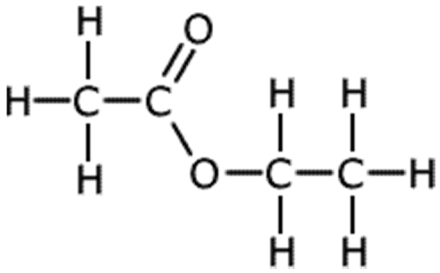

*Figure 23: Ethyl ethanoate*

The oxygen atom which is attached via a double bond to the carbon atom is disposed to bond with the carbon atom and this explains the stable nature of the compound. In the presence of water however the oxygen is disposed to dissociate from the carbon bond and bond with another oxygen. This power is referred to when explaining why the compound breaks down. The disposing towards metaphor is able to account for all of the different behaviours of the oxygen atom because, I suggest, it only amounts to an expression of nomological possibility. As long as there is some conceivable situation in which x will be part of the cause of y, then on Mumford and Anjum's account this makes it legitimate to say that x disposes towards y. We can claim x disposes towards y no matter how rare this occurrence is and regardless of other situations in which x disposes away from y. This expression of possibility might be helpful for a philosophical understanding of causation but it does not help chemists capture similarities or provide useful explanations.

Consider the sort of similarities that chemists want to capture. Their aim is to synthesise as much information from the reaction landscape as possible. Enzymatic reactions are particularly difficult to instantiate and require specific environmental conditions such as temperature, pressure and PH. Typically there is only a small window when these optimum conditions exist and in which the reaction will take place. Since similar reactions have similar optimum conditions the reaction landscape can be used to improve predictability. Mumford and Anjum's view might try to accommodate this by asserting that similar reactions will be associated with similar powers, however I suggest their account is unable to account for the complexity of the similarities at stake. In addition it contravenes the principle of explanatory

unification to state that 'the hydrolase enzyme disposes towards increased rate of reaction' as this is only the case under exceptional and often rare circumstances.

The effect of temperature on enzyme activity is particularly relevant. The ability of enzymes to catalyse reactions increases as temperature increases until an optimum temperature is reached. As a result we can state the heat energy disposes towards the instantiation of an enzymatic reaction. However once the optimum temperature is reached a further increase in temperature causes the enzyme to deactivate and its functionality to be reduced. The causal dispositionalist can accommodate this situation by maintaining that heat energy also disposes away from the instantiation of enzymatic reactions.

I suggest that the following assertions are unhelpful to chemical practice as more information is required for them to be useful to the formulation of predictions and explanations;

a. Heat energy disposes towards increased enzymatic activity
b. Heat energy disposes away from enzymatic activity

Mumford and Anjum would respond to this objection by appealing to the functions that govern how powers combine. They discuss this kind of overdose case when they introduced compositional pluralism. They state;

> 'It should be clear from overdose cases that simple addition is not the mode of composition because the resultant power fails to be doubled when we double the extent of the component powers. Hence, these cases count as non-linear composition' (Mumford and Anjum, 2011, 89).
>
> 'There are some cases that can be explained additively but we should accept a position of compositional pluralism: addition is just one among many different functions according to which causes compose' (Mumford and Anjum, 2011, 86).

Mumford and Anjum argue that functions govern how powers combine however they do not further elaborate on the nature of functions and add only that they should not be considered laws of nature (Mumford and Anjum, 2011, 99). Firstly, I

argue that given the crucial work functions do for their account and in particular, in capturing the kind of similarities revealed by the reaction landscape an ontological account of functions is required.

Secondly, even given an ontological specification of the mathematical functions by which powers combine, the causal dispositionalist account contains insufficient information to formulate successful predictions and provide useful explanations. I suggest that, in addition, all power attributions must come with a specification of the conditions under which that power is operative. For instance, enzyme E will dispose towards an increased rate of reaction R under conditions C.

I suggest that statements concerning powers disposing towards an effect are useless without additional disclaimers regarding

a. the required conditions
b. mutual manifestation partners
c. functions under which they combine in order to produce the effect.

In chapter 3, I criticised the entities - activities ontology on the basis that it did not contain enough possibility. I argue, in this case that causal dispositionalism contains too much possibility. It is both functions and a specification of the required environmental conditions that provide insight into which effects will come about and why. An attribution of a power should come with both, otherwise it appears that we can attribute a power to accommodate any situation and this is unilluminating from a scientific perspective.

In addition to the objections described above there is a further problem concerning whether Mumford and Anjum's account can capture the criteria explanatory unification which again results from the unconstrained nature of the disposes towards metaphor. As I described in section 2.2. the aim of my case study is to meet the demand from industry for more efficient reactions with higher yields. These reactions are then used in applications from medicine to dye making. I suggest that a causal dispositionalist account cannot provide the required explanations of

how these reactions are able to function in industry. This is again due to the unconstrained nature of the dispose towards metaphor

At several points in this chapter I have discussed Mumford and Anjum's example of the biological process describing the way in which the ingestion of arsenic causes death. I described how Mumford and Anjum attribute these causal powers to arsenic because each step in the causal process disposes towards the next and therefore, it is claimed, that the causal chain is transitive.

In the next section I provide other examples of causal chains that result from the application of enzymatic reactions in industry. I suggest that the application of the dispose towards metaphor fails to do justice to the importance of chemical manipulation and ingenuity and as a result is inhibited in the kind of explanations it can support.

Consider an industrial application of a hydrolysis reaction in which enzymatic reactions are used to convert biomass into biofuel as an alternative form of greener energy. As a result of the environmental and economic impact of fossil fuels investigations into this process have received substantial investment since the 1970s, however progress has been slow. The process begins with plants that are intensively grown to produce lignocellulosic biomass which contain cellulose, a long chain of glucose molecules with the formula $(C_6H_{10}O_5)_n$. This is converted into ethanol through a multistage process and is burnt to produce energy (Hendriks and Zeeman, 2008). Is it the case that cellulose disposes towards ethanol production in the same way that Mumford and Anjum argue that the oxygen disposes towards the lighting of the fire? I argue that the causal dispositionalist isn't able to point to a difference between these two processes and as a result the dispose towards metaphor ceases to be useful.

Cellulose is a polymer containing individual units which are intimately connected in a complex structure that is resistant to attempts to break it down. An important step in the process is the pre-treatment of cellulose in order to disrupt its naturally resistant structure. This pre-treatment involves mixing cellulose with

alkaline materials such as sodium, potassium, calcium and ammonia at specific temperatures and pressure. This causes the cellulose to swell which leads to a greater surface area for the enzymes to act on, it reduces the crystallisation and removes additional products such as dissolved hemicelluloses, lignin, and some unreacted inorganic chemicals. How should we interpret the process thus far?

*X1. Cellulose is disposed to swell and increase in surface area*

The next stage in the process is the hydrolysis of the cellulose to release shorter chains of soluble glucose sugar. The reaction is catalysed by cellulase which is a combination of enzymes that together lower the activation energy for the reaction to take place.

*X2. Swelled cellulose is disposed to react with water to form a glucose solution*

Finally the remaining water needs to be distilled via fermentation, the solution is heated and water is evaporated leaving ethanol and carbon dioxide.

*X3. Glucose is disposed to produce ethanol via distillation.*

If we assess these claims together we have;

*X1. Cellulose is disposed to swell and increase in surface area*

*X2. Swelled cellulose is disposed to react with water to form glucose solution*

*X3. Glucose solution is disposed to produce ethanol via distillation.*

*X4. Ethanol has the power to produce energy when burnt*

It looks like we have a causal chain much like the process by which arsenic disposes towards death in which one step causes the next and the transitivity of causation holds. However, to argue that transitivity holds in this case and so cellulose disposes towards the release of energy is not a helpful explanation from the perspective of practice. It ignores the huge amount of chemical ingenuity and manipulation that is required to *construct* the process from which biofuel is produced

from biomass. It is seems unnatural and counter intuitive to explain the process by stating that cellulose disposes towards energy given that the original cellulose molecules have extremely complex structures which resist attempts to break them down. The problem is that whilst the 'disposes towards' metaphor can be made to apply to any case it does so at the expense of becoming so weak it is unhelpful. I suggest that the statement 'cellulose disposes towards the release of energy' amounts to a statement of nomological possibility and this is not explanatorily useful.

## 5:6: Conclusion

My motivation for this chapter was the hope that the 'disposes towards' metaphor and the corresponding distinction between enabling conditions and causes might provide identity conditions for processes. If viable this would give us the processes appealed to in chapter 4 at a reduced ontological cost. I have shown that this is not the case and therefore commitment to an additional category of processes is required to accommodate the features of reactions discussed in section 4.4.

I began this chapter by outlining causal dispositionalism and the motivation for the distinction between causes and enabling conditions. I described how Mumford and Anjum want to retain the notion of the total cause whilst placing a limit on transitivity. An enabling condition is a part of the causal chain that does not dispose towards the next step in the chain thus constituting a break in transitivity. If this account is successful, the presence of enabling conditions in a causal chain could be used to individuate processes.

I showed that the causal dispositionalist account is not descriptively fit for purpose. It fails to give a descriptively accurate account of how processes are identified in practice because the physicochemical variables that might be construed as the powers at work in my case study act as causes of an event rather than causes of a process. I also argued that the causal dispositionalist underplays the role of perspective and interest dependence when identifying processes in practice.

I suggested the claim that x disposes towards y amounts to the claim that it is at least possible that x will be part of the cause of y; as a result causal dispositionalism contains too much possibility to capture similarity and give useful explanations. This problem could be overcome by a more through metaphysical account of the functions by which powers combine and the constraints under which they are operative.

# Chapter 6: A Metaphysics for the Classification of Reactions in Practice

## 6.1: Introduction

The aim of my thesis has been to investigate the most appropriate metaphysics for the classification of chemical reactions in practice. In this chapter I will outline my positive proposal. My thesis was motivated by the fact that the philosophy of classification pays little attention to the classification of non-entity like things yet the classification of reactions is a key component of chemical practice and is essential to the fruitful development of chemistry and its industrial applications. My approach has been to engage in a particular variety of naturalised metaphysics that is led by chemical practice, in order to provide a metaphysical framework that is fit for this practice.

My strategy has been to investigate which ontological components are required to accommodate the classification of reactions, in order to adjudicate between the accounts of classification outlined in chapter 1. I have already ruled out Ellis's strong essentialism on the grounds of the perspectivalism and interest dependence that directs chemical inquiry. On this basis I reject commitment to kinds of reactions where those kinds have essences. In chapter 3, I showed that commitment to dispositions is required to capture the classification of reactions in practice and in chapter 4 and 5 I showed that commitment to an extra ontological category of processes is also required. Since none of the remaining accounts of classification outlined in chapter 1 contain commitment to dispositions and processes, none are sufficient to accommodate the classification of reactions and I will introduce my own positive account.

My positive proposal is an ontological one concerning realism about the categories that are required for classification. I offer a two-fold proposal:

*Part 1a: Realism about processes as a distinct ontological category is necessary*

*Part 1b: Realism about the ontological category of entities and the ontological category of dispositional properties is also necessary in addition to the category of processes. None of these categories are on their own sufficient to capture the classification of reactions in practice*

*Part 2: A type of process is one where all token processes engage in the actualising of the specific potentiality that is associated with that type*

I will begin by discussing part 1 of my positive proposal. I've previously argued that a commitment to dispositional properties and processes are required and in section 6.2 I will address why an additional commitment to entities is also necessary. This discussion will distinguish my account from the recent account of processes provided by Dupré. In section 6.3 I will focus on part two of my positive proposal in which I appeal to the discussion of reactions throughout my thesis in order to outline the metaphysical picture underlying types of processes. In section 6.4 I will show how my 3-category ontology accommodates my case study and use this as an opportunity to flesh out the relations between the different ontological components. In section 6.5 I will offer some clarificatory remarks. I will highlight a further respect in which my account of processes differs from the account of processes offered by Dupré. I also address why I am optimistic about the scope of the ontological category of processes.

## 6.2: Commitment to entities

I suggest that to give a metaphysics of classification that is descriptively fit for purpose an additional ontological category of entities is required. This is the first way in which my account can be distinguished from Dupré's process ontology. Dupré rejects commitment to entities in favour of processes. He takes the world to be a

world of processes where it is the interaction of many processes working together that produces a level of stability. It is this stability that, according to Dupré, gives the illusion of entities. He suggests that we abstract away the relevant processes in order to identify a stable entity. On his view scientists identify stability in different scientific domains and so assert the existence of different and perhaps contradictory entities (Dupré 2012). It is the idea that processes are both fundamental and responsible for giving the illusion of stability that does the work in outlining the metaphysical framework behind Dupré's promiscuous realism.

Whilst I am ontologically committed to processes, I do not follow Dupré in taking processes to be fundamental. In chapter 4, I highlighted the distinction drawn by chemists between 'the thing that is changed' (the entity) and 'the change itself' (the reaction). The distinction is crucial in enabling chemists to meet the aims of their inquiry and should therefore be reflected in our ontology. This is evident through an assessment of the role of entities in the 3-stage classification process outlined in chapter 2. Stage 1 involves the identification of what chemists refer to as an activity of interest. This requires chemists to isolate a set of reactions that are known to be similar enough that a QSAR analysis can fruitfully be applied to reveal more fine grained similarities between the reactions. I showed in chapter 2 that each activity of interest is defined in terms of entities. For example,

*Hydrolysis reactions involve the breaking of a chemical bond of an entity by the addition of water.*

This approach to defining reaction is confirmed when we look to other examples of reactions as described in section 1.2:

- Neutralization Reactions are a special type of double displacement reaction that involve the reaction between an acid and base to form a salt and water.
  acid + base → salt + water
- Combustion Reactions occur when a hydrocarbon combines with oxygen to produce carbon dioxide and water.
  hydrocarbon + oxygen → carbon dioxide + water

- Polymerization is a type of chemical reaction that occurs when monomer molecules combine together to form polymer chains or three-dimensional networks.
- Photosynthesis reactions occur in all plant life. Carbon dioxide and water react with energy from the sun to produce glucose, oxygen and water
  $6\ CO_2 + 12\ H_2O + \text{photons} \rightarrow C_6H_{12}O_6 + 6O_2 + 6H_2$

Defining reactions in terms of a change in a particular entity is required if the classification landscape is to be produced. Therefore, treating entities as distinct from reactions is key to capturing similarity relations.

This point is confirmed by looking at the second stage of classification in which determinate values for physicochemical variables are, for each reaction, imported into a neural network to reveal the similarity relations that hold between the reactions. As I discussed in section 4.6.4, an appeal to practice reveals that these physicochemical properties are taken to be possessed by entities. For example, the property sigma electronegativity describes the 'ability of an atom to attract electrons'. Therefore, treating entities as distinct from reactions, i.e. as wholly present, and possessing a range of potentialities is important if we are to accommodate the second stage of classification and the identification of the similarity relations between reactions. The distinction enables chemists to meet the aims of their practice and should be reflected in ontology.

Commitment to entities is also required to meet the criteria of explanatory unification. In section 4.3. I described how chemists explain the features of reactions such as the rate of reactions and activation energy by appealing to entities. A given reaction involves many entities that each undergo a distinct reaction mechanism when they collide with the appropriate entity with sufficient energy. Explanations for why a reaction decreases in rate or how the rate of a reaction is affected by environmental conditions involve appealing to the relations between the entities involved in the reaction. Understanding these relations is crucial to making predictions about the behaviour of reactions. The fact that entities function in explanations about reactions suggests that realism about entities as a distinct

ontological category is required to meet the criteria of explanatory unification. It is for these reasons that, unlike Dupré, I retain ontological commitment to entities.

## 6.3: A Metaphysics for Types of Reactions

I have so far proposed a 3- category ontology consisting of entities, dispositional properties and processes. I suggested in chapter 4 and 5 that reactions fall into the ontological category of processes and throughout my thesis I have been concerned with illuminating chemists' treatment of reactions in practice. In this section, I will outline my key findings and use them to build a positive proposal for the metaphysics underlying my category of processes.

In section 4.2 I described the key differences between reactions and entities as they are treated in practice. I showed firstly that chemists introduce a distinction between entities and reactions whereby reactions are described as the means by which entities change. Chemists treat this as a fundamental distinction in chemical practice. In addition they identify reactions as being extended in time with distinct temporal intervals separating the start of the reaction from its coming to completion. This is in contrast to entities, which are wholly present at each point at which they exist.

In section 4.3 I discussed the way in which reactions and dispositions are treated in practice and concluded that the relationship between reactions and potentiality is unclear. I argued that there is something intuitively appealing about treating reactions as potentials. Reactions tend to be directed towards a certain end product just as a disposition is a potential for some 'F' to manifest. In addition, I showed that there is an absence or incompleteness associated with reactions; a reaction may be ongoing but is incomplete until the appropriate end product has been brought about. This is also the case with dispositions. Finally, reactions and dispositions bring about their own destruction, the reaction ceases to occur because the entity ceases to have that potential, it has been actualised.

However, I also described an opposing intuition in which reactions seem to be more than a mere potential, but also actual. They are described as a *happening* or a *coming to* be. I suggested in section 4.3 that the idea of a reaction as an active coming to be is supported by the fact that reactions can be interfered with, stopped or increased in rate whilst they are in actuality. This is an important aspect of chemical practice and is key to the manipulability of reactions in industry.

In section 4.4. I also showed that reactions involve multiple entities and dispositions and it is the relations between these component parts that are important for explanation and prediction. Finally in chapter 5 I showed that the way in which a reaction is distinguished from its context is dependent on the aims and interests of chemists conducting the investigation.

The characteristics of reactions that have emerged throughout my thesis can be summarised as follows. I will use these characteristics to build my account of the third ontological category of processes in which reactions fall.

1. Reactions are the means by which entities change
2. Reactions have temporal intervals
3. Reactions are not wholly present at any one time
4. Reactions are directed towards a certain end product
5. Reactions are incomplete until it is over, at which point it has brought about its own destruction
6. Reactions can be measured
7. Reaction can undergo change
8. Reactions have multiple arity
9. The identification of reactions from their context is dependent on the aims and interests of scientists

I suggest that the most fruitful way to proceed is to focus on the relationship between potentiality and actuality in a given reaction. I suggest that when we are led by chemical practice in this way we can give an account that meets all the criteria outlined above.

### 6.3.2: An Aristotelian Account of Change

My account is inspired by an Aristotelian account of change as developed by Coope (2009). I will begin by outlining this account of change and showing how it applies to reactions.

Aristotle asserts that things can change in terms of quality, quantity and place and attempts to provide a general account of change in which he is committed to the view that change is real (Physics III.1–3). According to Parmenides, change is not possible because something cannot come from what is not. Aristotle acknowledges this latter point but maintains that change is still possible. For Aristotle, change is real and possible so long as something is preserved through the change (Physics I.7–9). In the case of chemical reactions it is the constituent matter that is retained through the change even though its arrangement into particular entities might be altered.

Aristotle asserts that change is related to the notion of incompleteness however, he notes that there is a distinction between being incomplete and changing since it is possible for something to be incomplete and yet not undergo any change. Aristotle attempts to provide an account that characterises change as real, but also captures the manner in which it is incomplete thus showing the important relation between incompleteness and change. He gives a definition of change such that it is the 'actuality of that which potentially is, qua such' (Physics III, 201a10 - 11).

The first thing to note is that the potentiality associated with change is defined in terms of some specific actuality that isn't yet fulfilled, for example the *actuality of a lump of bronze qua potentially a statue*. Coope points to a problem with this view in that it allows for an interpretation of the actuality associated with change as merely the product of the change rather than the change itself. Coope argues that this is not a sufficient account of change and is not what Aristotle had in mind (Coope, 2009, 279). She asserts that Aristotle wants to capture the change as the becoming of the end product, for instance the change as the becoming of the statue, even if the statue isn't yet complete. Once the bronze has become a statue it is no longer

changing so it is counter intuitive to associate change with the production of the required end products.

This corresponds to our understanding of chemical reactions, a reaction is the means by which an entity changes and is therefore more than the end products of that change. Instead, the reaction is the active and directed unfolding over a number of temporal intervals until the end products are brought about via the reaction.

Coope utilises the concepts of potentiality, actuality and change to clarify Aristotle's position. She argues that what Aristotle has in mind is that change is the actualising of a potential for being. She states 'change is the actuality of what is potentially in some particular different state qua such i.e. the change that is becoming a status is the actuality of what is potentiality a statue qua potentially a statue' (Coope, 2009, 282). Coope comments that when Aristotle defines change as an actuality then he is suggesting change is real and is more than the existence of a potentiality but the becoming of the potentiality. Again, this corresponds to practice. Reactions are treated as real phenomena by chemists; they can be interfered with, made to go faster or slower and measured whilst they are in actuality. They are also real in the sense that they are deemed worthy of classification in their own right in order to achieve the aims of scientific inquiry.

In addition, Coope claims that by stating that change is the actuality of what is *potentially qua such* Aristotle highlights that the actuality associated with change is directed towards the fulfilment of a certain potentiality. It is a change in a certain respect. In the case of the bronze statue the actuality associated with the change is the actuality *insofar as it is merely potentially a statue*. This actuality is most fully actual prior to the bronze becoming a statue. When the bronze has become the statue then it no longer has the potential to be a statue and therefore the 'potential to be a statue' cannot be further actualised (Coope, 2009, 283).

I suggest that this account of change fits with the way in which chemists characterise and explain the initial stage of the classification process. The hydrolysis reactions from case study two all consist of the breaking of a chemical bond using

water. The water molecule is able to break the bond due to the polar charge on the $H_2O$ molecule, which attracts the shared pair of electrons in the reactants covalent bond. This is the defining feature of hydrolysis reactions and was used to identify a set of reactions sufficiently similar to engage in QSAR analysis and classification via neural networking.

Following Aristotle's' approach, we can identify types of reaction using the reaction type's corresponding potentiality where those reactions are considered to be the actualising of this potentiality. In the case of hydrolysis reactions we can identify the corresponding potentiality as *'a broken bond due to the presence of the polar change on a $H_2O$ molecule'.* It is the coming into actuality of this specific potentiality that all members of the type 'hydrolysis reaction' have in common. A hydrolysis reaction isn't just any change in the entities involved in the reaction, the change is the actualising of this particular potentiality. When the change has reached the designated end product the potentiality has been fully actualised, the change is complete and the reaction ceases to exist.

Aristotle develops his account of change by examining the process of building a house, he states 'the actuality of the buildable, qua buildable, is the process of building. For the actuality is either the process of building or the house, but when the house is, the buildable no longer is' (Physics 111, 201b9–11). Change is the process of 'coming to be' of a specific potential and it is the identification of this specific potential that distinguishes one reaction from another i.e. distinguishes reaction types. This point is further elucidated by examining the difference between the process of changing and the state that the entity it is in when it has the potential to change, but is not yet changing. Coope claims that this is achieved in virtue of the qua clause. In the case of the bronze and the statue it highlights a difference between the bronze being actual *qua bronze* and the actuality of the bronze *qua potentially a statue*. The bronze possesses the potentiality to be a status before it began changing but as Coope states, at this point, the potential was dormant, it didn't make a difference to the world or at least a difference with respect to the relevant end i.e. statueness (Coope, 2009, 282). It was only when the change began and this potential

began to be actualised that the potential made a difference to the world i.e. there is one more statue in the world.

This is a fruitful way to think about chemical reactions as it captures the distinction that is cited in chemical practice between entities and their properties on the one hand and reactions on the other, whilst retaining the notion that reactions are active and actual. Entities have the potential to engage in reactions and as I described in chapter 3 this is accommodated via a commitment to dispositional properties. Nonetheless, reactions involve something more than this, they involve the active coming to be of a potential. This actualising of the designated potential is extended over a temporal period and is not wholly present at any point at which it exists. Rather it is present at each time interval through which it is unfolding. Treating reactions as actual, rather than as potentials accommodates the feature of practice by which reactions are measured and can be interfered with.

We can now flesh out the metaphysics underlying the ontological category of processes. My strategy has been to appeal to the features of reactions to illuminate the category of processes. I have shown in chapter 4 that an additional ontological category of processes is required to capture the classification of reactions and therefore the best information we have about what a category of processes is like comes from our knowledge of reactions since we know that reactions fall within this category. However, I also hope to provide an ontological framework that is general and is applicable beyond this particular aspect of chemical practice. With this in mind, I have labelled this category 'processes' rather than 'reactions.' I expect that other phenomena, which are not chemical reactions will constitute processes and fall in this category. I will explore the scope of the category of processes section 6.5 below.

I now suggest that a type of *process is associated with the actualising of a particular potentiality*. The process is bounded by the dormant status of the potentiality before it has begun to be actualised and its full actualisation and therefore the destruction of that potentiality. An entity will have the potential to undergo many different processes and it is a matter for science to identify which particular potentiality corresponds to a given process. In other words it is up to

science to fill out the placeholders of my account of processes in each case, as below in the case of hydrolysis reactions. I can now flesh out part 1b of my positive proposal.

*1.b A type of process is one where all token processes engage in the actualising of the specific potentiality that is associated with that type*

For example:

*A hydrolysis reaction is the actuality of the potentiality 'to break due to the presence of the polar change on a $H_2O$ molecule'*

This allows us to accommodate the fact that reactions are a change and this change is real and active. The change is the coming to be of a potential although this may involve other changes such as the gain or loss of parts in the entities involved in the reaction. In addition the reaction is an unfolding that is directed towards the actualisation of a certain potentiality, in the example above the actualisation of any other potentiality would not constitute a hydrolysis reaction.

My account is also able to capture and explain the ways in which reactions are similar to dispositions in the sense that reactions involve a potential and thus, an incompleteness. However my account also allows for the required actuality that taking reactions to be dispositions forbids. By including commitment to processes and clarifying the relation between potentiality and actuality my account is not subject to the 'always travelling, never packing' objection against the dispositionalist account since it contains sufficient actuality. My account is compatible with the idea that reactions can be measured, interfered with and changed.

The metaphysical status of types of processes is therefore captured by taking them to be the temporally extended exchange from the potentiality to x to the actualisation of x; the process is the 'actualising of x'.

I will show in the next section that treating reactions in this way within the metaphysical framework of the 3-category ontology allows us to accommodate the

aims of chemical practice. I will also flesh out the relations that hold between the 3-catagories.

## 6.4: Capturing my Case Study

In chapter 2, I highlighted that the aim of the case study was to achieve a better understanding of the similarities that hold between the reactions undergoing classification in order to make the kinds of predictions that are required by industry. It is stated that;

> 'the similarity analysis of enzyme catalysed reactions can form the basis for searching for other enzymes that can catalyse a given reaction. Or, vice versa, for a given enzyme, different or novel reactions might be found that are catalysed by the same enzyme' (Sacher, Reitz, Gasteiger, 2009, 1525).

In particular, I described the desire to provide a 'definition of similarities between reactions' (Sacher, Reitz, Gasteiger, 2009, 1525).

I showed in chapter 2, that the information that is required to manipulate reactions for industrial purposes is also included in this definition of similarities revealed on the reaction landscape. For example, hydrolysis reactions form part of complex industrial processes that require continual management with the reaction conditions monitored and adjusted to produce the required yield and improve efficiency. Consider one of the reactions undergoing classification in case study 2. Below is a general reaction equation for the reaction type whose members are catalysed by enzymes from the EC 3.2.1.d subclass.

**EC 3.2.1.d**

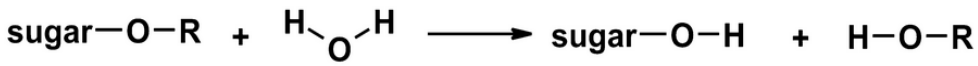


*Figure 24: General reaction equation for the reaction type whose members are catalysed by enzymes from the EC 3.2.1.d subclass*

In this reaction the entities involved in the reaction are sugar molecules, oxygen and hydrogen with the R standing for an additional group that is not involved in the reaction centre.

The overall reaction itself consists of many instances of the same reaction mechanism illustrated above over a temporally extended period. It is the instantiation of these reaction mechanisms that constitutes the reaction as a whole. I showed that due to the restricted arity of entities and dispositions reactions cannot be reduced to entities and dispositions. Rather, an account of properties of reactions such as the rate of reaction requires an analysis of the relations that hold between the many entities involved in the reaction as a whole. I have not addressed whether, generally speaking, reaction mechanisms can be accounted for in terms of entities and dispositions. Nonetheless, this is irrelevant to my argument that a category of processes is required to capture the classification of reactions. If it turns out that reaction mechanisms cannot be captured by entities and dispositions then they will fall in the category of processes alongside reactions themselves.

To return to the example above, all reactions of the type EC 3.2.1.d have in common that they involve the breaking of an O- glycosidic bond in the presence of water. The O- glycosidic bond is a covalent bond involving oxygen that links a sugar molecule to another group R. This constitutes the definition for this type of process and we can use this definition to isolate the corresponding potentiality. The reaction type EC 3.2.1.d is the actualising of the potentiality *to break an O- glycosidic bond in the presence of water.* It is important to clarify that this is the general potentiality associated with the reaction as a whole. Each entity involved in the reaction has a number of dispositional properties and the actualisation of these dispositional properties is associated with a particular reaction. According to chemists they 'encode the reaction' though reactions cannot be accommodated in terms of the manifestation of these dispositions due to the restricted arity of dispositions.

The 'actualising' of the potential associated with the reaction as a whole can be increased or decreased in speed by manipulating the environmental conditions. This is important to industry because to keep a reaction running at a reduced rate is

more efficient than stopping and starting a given reaction. The 'definition of similarities' referred to above gives chemists the resources to control the 'actualising of the reaction'. For example, there are 180 enzymatic falling within sub group EC 3.3.2.d and each of these reactions exhibits a high degree of similarity to each other. The particular degrees of similarity are revealed in the reaction landscape. One member of this group is the enzymatic reaction EC 3.2.1.4 which involves the enzyme Cellulase (otherwise known as 1,4 β-endoglucanase) and which is used to produce glucose on an industrial scale. Due to the importance of this reaction in industry numerous investigations have been carried out into the optimal conditions for the cellulose enzyme to operate (Yennamalli, 2013). It was found that activity was optimised when the substrate was treated with an alkali at PH 5.5. and when the reaction occurred at 30˚C. This information is also used to predict the optimum condition for reactions that appear close to EC 3.2.1.4 on the reaction landscape.

In order to accommodate chemists' attempts to manipulate reactions in this way we must treat each reaction as a single unified being falling in the ontological category of processes. This accommodates the fact that reactions are treated as retaining their identity throughout the 'actualising of the designated potential' even though the rate at which the actualising is taking place might change. The reaction itself changes and as well as it being the means by which a change is brought about in the entities (O – Sugar – R) and ( O-H-O) in the diagram above. The exact relationship between environmental conditions and the rate of reaction can be described using the Arrhenius reactions and used to make quantitative predictions. This involves the identification of empirically determined properties of each reaction such as rate coefficient and frequency factor. These are the properties of the reaction taken as a whole and again this suggests that the reaction be treated as a separate ontological category in order to support chemists' need for manipulability.

I described in chapter 2 that the aim of the inquiry was a better understanding of the similarities that hold between the reactions in order to make predictions as required by industry. In particular I described how chemists wanted to 'explore the reasons for the bonds being broken' (Sacher, Reitz and Gasteiger, 2009, 1525). It is

dispositional properties that do the work in supporting predictions and explaining which bonds will break.

In the reaction equation described in figure 24 above, all of the entities that break or make bonds during the reaction are identified as the reaction centre. This includes the O-R bond (which is also attached to the sugar molecule) and the O-H bond in the water molecule. For each of the 180 sub types of reactions that fall within this group, the reaction centre is identified and corresponding data describing each reaction centre retrieved. This data concerns the dispositional properties associated with the reaction centre.

The reaction was premised on the notion that the presence of certain dispositional properties over others corresponds with the instantiation of certain reactions. For example, when taken in isolation from other factors, an entity (or reaction centre) with a particularly high value for polarity is more likely to undergo a hydrolysis reaction in the presence of water.

The investigation into the classification of chemical reactions was premised on the notion that entities with similar values for each dispositional property will each undergo a similar reaction mechanism and therefore produce similar reactions. In addition, a difference in physicochemical variables or dispositional properties is indicative of different reaction mechanism and therefore different bonds being broken. The production of the reaction landscape using dispositional properties had by entities supports more general predictions concerning which enzymes are most likely to catalyse which reactions on the basis of reaction similarity. Therefore dispositional properties are essential to meeting the aims of classification of demand from industry.

In addition the potentiality associated with predictive statements about whether the reaction will occur requires commitment to dispositional properties. This is because the potentiality cannot be grounded in the reaction itself as that reaction hasn't come into existence. This is in contrast to the ontological commitment to processes, which I suggested above is required to make predictions

concerning the environmental conditions under which an enzyme will reach its optimum level of activity when the reaction is ongoing.

I suggest that the relations between the three ontological components is captured by stating that dispositional properties play the role of anchoring entities to processes. According to my notion of anchoring, the reaction process that takes place is dependent on the presence of those determinate values for the dispositional properties had by entities. Physicochemical properties of the reaction centre correlate with which reaction will occur. It is important to note, however, that the reaction isn't fully determined by physicochemical variables and chemists actively investigate how the rate of reaction can be altered when it is underway.

This notion of dispositional properties anchoring entities and processes also applies to the completion of the reaction. Throughout the course of the reaction, the entities that are undergoing changes to their identity will manifest different dispositional properties. These properties direct the course of the reaction and variation in these dispositional properties will equate with variation between reaction processes. Those properties that manifest themselves during the reaction process will determine which entities are formed as final products of the reaction i.e. which intermediate products of the reaction have the greater electron attracting power will determine which new bonds are formed.

An account of dispositional properties as anchoring entities to processes represents an advantage of my ontology over the entities – activities ontology. MDC are unable to explain why an entity engages in a particular activity at a given time. Whilst MDC might state that the entity functions as part of a mechanism, they cannot explain 'in virtue of what' the entity functions or takes part in that mechanism. I am able to explain the relation between entities and processes in terms of dispositional properties. Entities take part in particular processes as a result of the manifestation of their potencies. Whilst entities, dispositions and processes are clearly related none can be reduced to the others in a way that is descriptively fit for purpose. I showed in chapter 3 that dispositions are required in addition to entities and in chapter 4 that

processes are required due to the problem of arity. I also showed that processes cannot be reduced to entities and dispositions due to the problem of potentiality.

The relations between the three ontological categories are also captured in my definition of a process. A particular reaction process is itself defined as a manifestation of a certain disposition that is had by the entities involved in the reaction. As a result of the reaction process coming to completion that potentiality is destroyed and the entities produced at the end of the reaction will have different potentialities in virtue of the change that has just occurred. Each of the three categories are therefore ontologically on a par but intimately related.

## 6.5: Clarifications

I previously stated that my ontology of processes is distinct from the account provided from Dupré (2012) because I also commit to a category of entities whilst Dupré takes processes to be fundamental. However, it's also interesting to assess important differences in our treatment of processes. Dupré defines a process as 'something that must continue to change in order to continue to exist' (Dupré, 2012). His definition is similar in sprit to the one I have outlined. On my view, a process must be actualising a specific potential in order to continue to it exist. When this 'actualising' has come to completion, the potentiality has been destroyed and the reaction has come to completion. In this sense, Dupré is correct to say processes must be continually changing to exist since it is feasible to equate this changing with actualising. However, my account of a process is more illuminating that Dupré's because it captures the directedness of processes and as a result is able to distinguish the different types of process that chemists are interested in. Dupré is not concerned with this because he does not commit to natural kinds of process or deal with the classification of processes. He is interested instead in outlining the metaphysical picture behind his promiscuous realism with respect to the classification of entities. Given the importance of the classification of reactions in practice, Dupré's account is worse off for not addressing this aspect of practice.

One aspect of Dupré's account that I retain is his perspectivalism. Within the remit of chemoinformatics chemists are primarily interested in solving industrial problems and it is this that directs their inquiry. As I discussed in chapter 5, this interest-dependentness is determined by the chemist's inquiry. Chemists interested in hydrolysis reactions will describe the breaking of a bond with water and the formation of the new bond as the end point of the reaction. In chapter 5, I also discussed an example in which chemists interested in pancreatic digestion will specify a more complex chain of reactions in which a hydrolysis reaction forms a part. This process involves the breaking of a bond using hydrolysis to form amino acids, a reaction with a substance known as glucogon and the polymerisation of the amino acids to form more useful proteins. Nonetheless, biochemists take these component parts to form one distinct process.

I suggested in chapter 5, that this interest-led individuation of processes is problematic for causal dispositionalists such as Mumford and Anjum, given that they reject the notion that epistemological concerns are relevant to matters of ontology. Nonetheless, this perspectivalism is compatible with a non-essentialist but realist account of processes such as mine. My account is non-essentialist because I do not commit to the claim that processes have essences in order to accommodate this perspectivalism. All that is required for realism about types of processes is that the unity associated with the whole process permits inductive inferences i.e. the similarities hold over the process as a whole as is the case with those revealed by the reaction landscape reaction such as velocities and activation energies.

A potential objection to my account concerns its applicability beyond the field of chemoinformatics and the case studies described in chapter 2. I suggest however, that there is reason to be hopeful about the scope of my account when we note the development of Basic Formal Ontology (BFO) by Smith (2012). This is a top level ontology which has been embraced across scientific disciplines with the aim of enhancing scientific practice by allowing unification across separate domains of inquiry. The ontological framework offered by BFO is similar to my account in that it

consists of three ontological categories that map onto the categories I have committed to.

The framework was developed to bring order to the terminology used by scientists across different disciplines. In this sense it is a domain neutral ontology (Seppala, Smith Ceusters 2014). It is stated that;

> 'Numerous domain ontologies use the Basic Formal Ontology (BFO) as an upper level reference ontology. BFO is a realist, formal and domain-neutral upper level ontology that is designed to represent at a very high level of generality the types of entities that exist in the world and the relations that hold between them [1-3]. BFO is intentionally very small, since it is intended to provide only the most basic building blocks for the construction of domain-specific ontologies at lower levels.' (Seppala, Smith Ceusters 2014).

BFO differs from my account in the sense that it is domain neutral and is instead aimed at providing unification across domains whilst my account is built by looking specifically at the details of inquiry within a domain.

BFO was developed as a result of the rapid growth of computer processing techniques required to analyse the large volumes of data becoming available to scientists. In order to better cope with this data, scientists tended to develop their own domain-specific organisational systems that categorised data in a way that was relevant to them and that best suited their needs. The idiosyncratic way in which this data is organised by different groups of scientists working within different domains often led to difficulties (Smith, 2012, 463). For example, it is unhelpful to build a scientific database using terms that are domain specific as this can mean that the data is inaccessible to neighbouring domains to which it may also be useful. Additionally, the meaning of terms or the terms themselves may change over time causing confusion and inhibiting scientific progress. BFO provides a domain neutral ontology that helps scientists better organise data by tagging it in a way that is useful across scientific disciplines and in such a way that searches of large volumes of data can be easily conducted. (Smith, 2012, 463).

BFO serves as a starting point for the production of over 100 domain specific ontologies across chemistry (Batchelor, 2008) biology (Smith, Köhler and Kumar,

2004) and biomedicine (Ceusters and Smith, 2006) to environmental science (Bittner, Donnelly and Smith, 2009) and computer science (Smith, 1998). It provides 'formal ontological architecture' via a set of general terms and relations that appear in each of the 100 ontologies covering distinct scientific domains. BFO includes only 34 terms including; 'process' 'object' 'function' 'role' 'disposition' 'generically dependent' and 'continuant fiat boundary' (Smith, 2012, 469). Each term included within the ontology must either be primitive or derivable from a term that is itself primitive. The most successful scientific ontology in use is the gene ontology which comprises 30,000 terms that correspond to types and subtypes of biological processes, molecular functions, and cellular functions.

The key point to note for present purposes is that BFO is similar to the ontology I have developed through the course of my thesis. BFO contains three distinct ontological categories each of which is divided into types and tokens as outlined below.

The first category is the category of 'independent continuants' which contains objects such as cells, humans or receptors. This resembles my category of entities. Secondly, there is the category of dependent continuant which is akin to my dispositional properties and require things to exist for their instantiation. Examples of dependent continuants on BFO are the power of the vegetable to rot, or the function of the canal to enable transportation (Grennon and Smith, 2004, 150). Also included in this category are qualities such as shapes, sizes, and elevations (Grennon and Smith, 2004, 151). The third category of occurrents is akin to my category of processes. An example of an occurrent on BFO is the eroding of the rock, tornadoes or troop movements in an army (Grennon and Smith, 2004, 154). It is claimed that continuants and occurrents mark two ways of existing; for an occurrent there is a temporal interval in which it occurs and for a continuant there is a temporal interval in which it exists. Occurrents also require independent continuants in order to exist.

Whilst it is beyond the scope of my thesis to offer a comparison between my account and BFO, the similarities in the 3 ontological categories and the widespread

application of BFO in other scientific domains suggest that my ontology has the potential for a broad scope.

To conclude, I propose a 3-category ontology consisting of entities, dispositional properties and processes. I've given a metaphysics for types of processes where a type of processes is defined as the actualising of an empirically specified potentiality. Types of reactions as identified in classification are also types of process.

## 6.6: Conclusion

In this chapter I have outlined my positive account for a metaphysics of classification of chemical reactions in practice. I proposed a 3 category ontology consisting of entities, dispositional properties and processes where reactions fall into the category of processes.

I outlined the metaphysics underlying my category of processes by appealing to an Aristotelian account of change that captures the relationship between potentiality and actuality. On my account a type of process is one where all token processes engage in the actualising of the specific potentiality that is associated with that type. I showed how my proposal captures the way in which reactions are both similar and different to dispositions.

I then fleshed out my case study in light of my positive proposal and discussed the relations that hold between the different ontological components such that dispositions anchor entities to processes and vice versa.

Finally I showed two ways in which my account is different to the account of processes offered by Dupré. Unlike Dupré, I remain committed to entities. In addition, my account of processes is similar in spirit to Dupré's but goes further by fleshing out the relation between potentiality and actuality in the context of scientific examples. My account also has the advantage over Dupré that it can accommodate the types of reactions revealed during classification. I ended this

chapter by offering a reason to believe my account has scope to be applicable beyond this particular aspect of scientific practice

# *Conclusion*

The aim of my thesis was to provide an appropriate metaphysics for the classification of chemical reactions in practice. My thesis was initially motivated by the observation that chemical reactions are classified into types and subtypes. Common types of reactions include acid - base reactions, combustion, oxidation, isomerization, and hydrolysis reactions. I noted that there has been an extensive literature on the classification of chemical entities with the periodic table remaining the paradigmatic example of a natural kind, however a philosophical account of the classification of reactions has been largely neglected. I noted that the most likely reason for this is 20$^{th}$ century philosophy's preoccupation with objects and entities as the building block of natures as opposed to any fundamental difference in the way chemists' treat classifications of entities and classifications of reactions.

My aim in chapter 1 was to given an account of the approaches to classification in the philosophy of science that might be applicable to the classification of reactions. In the chapters that followed I employed a highly naturalistic methodology that was led by scientific practice, in order to learn more about the nature of reactions, their classifications schemes and their place within scientific inquiry. The aim was that this analysis would provide the means for analysing which of the accounts of classification discussed in chapter 1 would best suit the classification of chemical reactions in practice.

In chapter 1 I discussed conventionalism about classification, semantic essentialism, metaphysical essentialism as well as Quine, Boyd and Dupré's varieties of weaker realism. I argued none of these accounts at present, have the resources for capturing the classification of chemical reactions however, several accounts offered hope for fruitful development in this respect. For instance, Ellis's scientific essentialism offers a place for kinds of processes in his ontology, Boyd utilises the

notion of a causal mechanisms in his account of natural kinds whilst Dupré argues that processes are themselves more fundamental than entities.

In chapter 2 I turned to chemical practice. It was beyond the scope of the thesis to look at all instances of chemical classification so I chose to focus on the classification of reactions within the domain of chemoinformatics. Chemoinformatics is a fairly new methodology that was developed to utilise the large volumes of chemical data that is now available for analysis. The approach is driven by empirical data and the desire to understand and manipulate it. Reaction classifications produced using chemoinformatics are intended to solve real world problems and improve and develop the application of chemistry in industry for example, in drug discovery. Taken together these two reasons mean that focusing on those classifications of reactions within chemoinformatics, allows me to best avoid antirealist accusations that the classification of reactions is for the purpose of more efficient storage or effective teaching and should not be taken as seriously as the classification of entities. Appealing to chemoinformatics suggests that, for at least some classifications of reactions, there is reason to believe this is not the case.

In chapter 2 I fleshed out the criteria that a metaphysics of classification must meet to capture my case study. I referred to this generally as being descriptively fit for purpose. By this I had in mind that it should be consistent with and led by the aims and interests of scientific inquiry and facilitate scientists meeting the end goal of their investigation. The aim of the case study discussed in chapter 2 is a growth in the knowledge of different enzymes and an understanding of how this scientific knowledge can be manipulated to produce greater predictive accuracy.

In order to be descriptively fit for purpose I argued that a metaphysics of classification of reactions must meet three more specific criteria. Firstly, it should be descriptively accurate or rather descriptively accurate enough. This means that it should not contain claims that are inconsistent with theoretical knowledge. Abstractions and approximations are permitted in so far as they do not inhibit the predictive ability. There are two specific features of the methodology of classification with which a descriptively accurate metaphysics must be consistent with.

Firstly, the classification process uses higher level reactions as heuristic devices. An initial type of reaction is identified on the basis of theoretical knowledge and then a more refined classification of token instances of that reaction type is produced. This second stage of classification has been the focus of my investigation. Here, QSAR is used to identify the lower level properties that are responsible for the instantiation of reactions. This data is then input into a neural network to produce a 2- dimensional classificatory scheme representing the similarity relations that hold between the reactions. I discussed how the purpose of QSAR is to provide a unified account of the reaction in terms of the most appropriate lower level structural properties. In addition a difference in the instantiation of a reaction is indicative of a difference in the structural properties of the entities involved in the reaction.

Secondly, I noted how neural networking is used to organise the data in a 2-dimensional reaction landscape. I concluded that in so far as chemists are interested in using these classifications to make predictions, then the 2- dimensional representation takes priority since this reveals the types and degrees of similarity that hold between individual token reactions as well as clusters of reactions.

In order to be descriptively fit for purpose, a metaphysics must also capture the similarity relations that hold on a reaction landscape. If chemists identify that two reactions are similar then this can be used to make predictions about how the reaction will behave under a variety of conditions. In chapter 2 I argued that the kinds of similarities that need to be accommodated by our metaphysics when making predictions are as follows:

1. Reactions falling within the same cluster will tend to be activated by the same type of enzyme.
2. Reactions falling within the same cluster will tend to require a similar amount of activation energy.
3. Reactions falling within the same cluster have a tendency to be affected by environmental conditions such as temperature, pressure and concentration.
4. Entities with similar physicochemical properties will tend to engage in similar reactions.

In addition to these direct statements regarding how a reaction will proceed there is another variety of similarities that need to be accommodated by our metaphysics. These are revealed by the classification of enzymatic reactions and are shared by the members of a particular subclass or cluster. These similarities include:

5. Number of bonds broken during the reaction.
6. The change in bond order (i.e. single bond to double bond).
7. The consecutive vs. simultaneous breaking of bonds.
8. Substructure of the reaction i.e.
    a. Part of the entity of which the reaction is centred.
    b. Substances released during the reaction in addition to the desired product.

These similarities are not directly used to formulate predictions but instead are added to the bank of theoretical knowledge and promote a better understanding of reactions. This leads to the third requirement on our metaphysics. A metaphysics that is descriptively fit for purpose is one that promotes explanatory unification. More specifically, it promotes better explanations of why reactions behave the way they do, giving chemists the resources to more successfully manipulate chemical knowledge to meet the aims of their inquiry.

At this point in my thesis I was able to make some initial claims about the kind of account of classification that is appropriate to the classification of reactions. I suggested that we can rule out a constructivist account of classification. The reaction landscape is successful in supporting inductive inferences regarding the way in which reactions proceed, which proteins will act as catalysts and the optimum conditions by which the reactions proceeds. We can appeal to the no miracles argument and assert that the best explanation for the successful predictions made on the basis of similarity relations is that those similarities exist in nature. In addition, in so far as the investigation is led by human interests it is led by a desire to better understand a particular chemical phenomenon.

A discussion of my case study also revealed that strong essentialism of the sort outlined by Ellis is also inappropriate for the classification of chemical reactions. According to Ellis, kinds of reactions have essences. The reaction landscape is produced with a specific research interest or investigation in mind and this dictates the particular reactions inputted into the reaction landscape. In addition, the similarity relations revealed on the landscape are themselves dependent on the reactions that are inputted. Therefore, whether two reactions are deemed to be similar depends on the other reactions under investigation. This perspectivalism is a reason to reject strong essentialism about kinds of reactions.

I concluded that a weak realist account of the types of reactions revealed by the classification scheme would be most appropriate. In order to evaluate which, if any, of the remaining accounts were suitable, my strategy was to determine which ontological components are required for our metaphysics to be descriptively for purpose. This could then inform my choice between the accounts of classification and the ways in which they need to be developed to accommodate reaction classification in practice.

I began by looking in chapter 3 at the mechanisms literature within the philosophy of science. There were two motivations for this; firstly we intuitively think of reactions in terms of their reaction mechanism and secondly MDC's account of mechanisms is committed to entities and activities, and activities as referred to by chemists are also a key part of my case study.

I began chapter 3 by giving an account of the term activity as it is used by MDC and then compared this with the way the term is used in my case study to ensure the two were consistent. I concluded that both take activities as distinct beings in their own right and as distinct from the entities which engage in them. They also both take activities to be a kind of change. Thirdly, they agreed that activities tend to involve more than one entity.

I hinted at a problem for the entities – activities ontology's ability to capture my case study by showing that the properties on which classification is based can be

characterised as dispositional properties as well as activities where there is no obvious reason to prefer one characterisation to another. I developed this point by asking whether a characterisation in terms of activities could do the work that was required of it. I began by suggesting that the entities – activities ontology must be able to ground the kinds of possibility statements that are used to formulate predictions using the reaction landscape.

For activities to do this work they must have a modal quality, I then engaged in an interpretative project examine the modal nature of activities. I concluded that even if MDC intend to give a modal reading to activities, additional commitment to dispositional properties is also required to capture certain types of possibility statements. Commitment to dispositional properties also accommodates the way potentiality is treated in chemical practice.

I suggested that commitment to dispositional properties improves explanatory unification by providing a way of anchoring activities and entities together. Entities engage in a certain reaction as a result of the dispositional properties that they possess however, the reaction then produces a new entity with a new set of dispositional properties. Therefore commitment to dispositional properties gives a better understanding of the relationship between entities and activities. I concluded that the physicochemical variables on which classifications are based fall into a distinct category of dispositional properties.

Having established that dispositions are a required ontological element, in chapter 4 I went on to investigate whether an entities – dispositions ontology is sufficient to accommodate chemical practice. I began by comparing the treatment of reactions in practice to the treatment of entities and the treatment of dispositions (physicochemical variables). The aim was to better understand the metaphysics underlying types of reactions.

I argued that reactions are different from entities in the sense that they are treated as the means by which entities are changed. Also, unlike entities they are

extended along distinct temporal intervals and are not wholly present at any one time at which they exist.

My comparison of reactions and dispositions is particularly interesting as it reveals some keys similarities as well as important differences. For example, both reactions and dispositions are directed towards a designated end point and are associated with an incompleteness. In addition, both reactions and dispositions bring about their own destruction by attaining this completeness. However I also showed that characterising reactions as dispositions neglects part of the story about reactions that is essential to classification into types. Treating reactions as dispositions neglects the fact that reactions constitute an unfolding or a happening that extends across distinct temporal intervals and is measurable at each point at which it occurs. Secondly, treating reactions as dispositions doesn't reflect the fact that reactions are active, ongoing and capable of change.

I also showed that the classification of reactions cannot be accommodated by treating reactions as collections of entities and dispositions. This is because the restricted arity of dispositions means they cannot be used to give an account of properties of the system. These properties such as reaction velocity and activation energy result from the interactions between the many entities and dispositions involved in the reaction process. It is the relations between these component parts that are used for making the kind of predictions and providing explanations concerning the behaviour of reactions. Treating reactions as distinct existences that have properties attributed to them is also in line with how they are treated in practice. Law-like generalisations are taken to apply to types of reactions whilst the entities and properties involved in the reaction are abstracted away.

I concluded this chapter by suggesting that a distinct ontological category is required to accommodate reactions. I labelled this category 'processes'.

In chapter 5 I investigate the possibility that the causal dispositionalist account can provide identity conditions for processes at no extra ontological cost in addition to dispositions.

I introduced the 'disposes towards' metaphor and the corresponding distinction between enabling conditions and causes. I showed that according to the causal dispositionalist, enabling conditions place a limit on the transitivity and as a result are able to individuate causal processes.

I then argued that the causal dispositionalist account is not descriptively fit for purpose. It fails to give a descriptively accurate account of how processes are identified in practice due to a discrepancy between the *causing of an event* and the *causing of a process*. I also argue that the causal dispositionalist underplays the role of perspective when identifying processes in practice.

I show that the causal dispositionalist account fails to meet the capture similarity relations and promote explanatory unification due to the dispose towards metaphor being vague and unconstrained. Any possible situation can be explained by the presence of a particular power. I argue that the attribution of powers should come with a specification of the various conditions under which that power might be operative. Mumford and Anjum appeal to functions that govern powers but tell us they should not be considered laws of nature. A more detailed account of the ontological status of function is also crucial if the causal dispositionalist account is to be descriptively fit for purpose.

Finally, in chapter 6 I outlined my positive proposal for a metaphysics for the classification of chemical reactions in practice. I suggested that ontological commitment to entities, dispositional properties, and processes is required if my account is to be descriptively fit for purpose. I added that on my account:

*A type of process is one where all token processes engage in the actualising of the specific potentiality that is associated with that type*

For example:

*A hydrolysis reaction is the actuality of the potentiality 'to break due to the presence of the polar change on a $H_2O$ molecule'*

I showed how my proposal captures the way in which reactions are both similar and different to dispositions. A reaction is a manifestation of a particular potentiality that brings about its own destruction when the reaction comes to completion and the potentiality no longer exists. In addition, by characterising a reaction as the actualising of a potentiality I am able to capture the way in which it is active, can be interfered with, measured and changed in practice.

I've also suggested that my three ontological categories are intimately related. Entities engage in certain processes as a result of that entity possessing certain determinate dispositional properties. In addition the unfolding of the process produced entities with further dispositional properties.

I ended by remarking on the separate development of Basic Formal Ontology as a top level ontology which is intended to unify the way in which scientific terminology is used across different scientific disciplines. Basic Formal Ontology contains three ontological categories of independent continuant, dependent continuant and occurrent which match onto my category of entities, dispositional properties and processes. Since Basic Formal Ontology has been embraced across a range of scientific disciplines and used to construct over 100 lower level domain specific ontologies I suggest that there is reason to believe my ontology will be applicable beyond the classification of chemical reactions.

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