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# Extending Kitcher's Account of Reduction to Other Special Sciences: A Consideration of Organic Chemistry and Quantum Mechanics

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Extending Kitcher's Account of Reduction to Other Special Sciences: A Consideration of Organic Chemistry and Quantum Mechanics

Kitcher's essay, "1953 and All That: A Tale of Two Sciences," argues against reductionism by showing how explanations of classical and molecular genetics are autonomous and how one cannot be substituted for the other without losing accuracy and clarity (Kitcher 972). It can be shown that Kitcher's argument is true outside of biology by detailed consideration of examples from other sciences; the one considered here will be a perceived reduction of organic chemistry to quantum mechanics. The example of organic chemistry and quantum mechanics shows that autonomy of the two explanations stems from their different objectives, purposes, and methods. The autonomy not only enhances explanatory powers of the theories, it also cannot be argued to have metaphysical connotations by employing Nancy Cartwright's view non-existence of physical laws.

Organic chemistry describes reactions characteristic of carbon compounds based on empirical evidence from experimentation. It often makes use of reaction mechanisms, that is, graphical representations of chemical reactions that are intended to predict the outcome and explain why a reaction undergoes a certain pathway. As already mentioned, one of the justifications for a mechanism is experimental: The identity of a product of a reaction can be verified using spectroscopic techniques.<sup>1</sup> However, mechanisms do not only identify the product. They also show the entire pathway by which the product is

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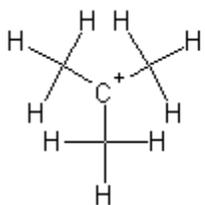
<sup>1</sup> Spectroscopy will be considered adequate verification of a reaction outcome throughout this paper. It is not the same as direct, unaided observation, but the justification of spectroscopy is not the topic of this paper.

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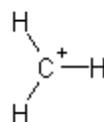
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obtained, often comprising of a multitude of intermediate steps. The intermediate species are usually short-lived, and thus, the empirical evidence for their identity is significantly weaker. The common justifications for reaction mechanisms in the realm of organic chemistry are the differences in energy between the products and the intermediates. Under usual conditions, all systems tend to lower their internal energy. The intermediate species are high energy, and they can collapse or combine, lowering their energy and driving the reaction forward.

Take these two systems for example:



a) 3° carbon cation



b) methyl cation

They both show carbon cations,<sup>2</sup> high-energy molecular ions that could play the role of intermediates in a reaction. The chemistry of (a) is radically different than (b) because (b) is much higher in energy. It is so energetic, in fact, that it never forms spontaneously under normal conditions. The accepted explanation of this difference in organic chemistry is that in system (a), the positive charge of carbon, can spread over a larger volume of space through the three carbon-carbon bonds. Thus, the effect of charge is delocalized, and the system has an overall lower energy. In system (b), the charge is

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<sup>2</sup> Positively-charged ions.

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localized on carbon. Because hydrogen atoms are very small, the charge cannot propagate over a large volume of space. The charge is point-localized, and thus, the system has higher energy.

This explanation is considered perfectly valid in organic chemistry. It makes at least two important assumptions:

1. The Lewis structures<sup>3</sup> shown in (a) and (b) are accurate representations of real molecular entities.
2. Effects of charge localization/delocalization are universally true and do not need further justification.

In the specific case of (a) and (b), assumption 1 has two additional assumptions embedded in it: it assumes that Lewis structures in general represent real species, and it also assumes that carbon cations exist. After all, no chemical company offers carbon cations in its catalog; they form only in a context of a chemical reaction, and being too reactive, they cannot be isolated from a reaction mixture.

All of those assumptions are justified but not in the realm of organic chemistry. The discipline that provides justification is quantum mechanics, and all organic chemists recognize that their field is very indebted to the development of quantum mechanics. Quantum mechanics describes, mathematically, the elusive concept of energy. Using complicated, theory-laden models, it is possible to calculate relative energies of (a) and (b) and to show that (b) is indeed higher energy than (a). Also, it is possible to make a

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<sup>3</sup> Lewis structures are symbolic representations of molecular structure. They consist of atomic symbols and lines to represent bonds between atoms. Electrons are represented as either dots or lines.

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law-like generalization about charge delocalization and energy that organic chemistry assumes to be true. Thus, assumption 2 is directly validated by quantum mechanical calculations.

At the same time, however, quantum mechanics is a radically different kind of explanation. Lewis structures do not have any meaning in the realm of quantum mechanics. In fact, they are shown to be utterly misleading. The covalent<sup>4</sup> bond graphically represented as a line between two atoms is really a cloud of shared electron density, and even more importantly, electrons are far from being localized anywhere. Electrons have wave-like properties, and in quantum mechanical models, they are recognized to have a form of a cloud of electric potential that spreads over a mathematically defined volume around nuclei. The shape and size of the cloud can be precisely calculated from Schrödinger equations, and it constitutes the atomic or molecular orbital. The bottom line is that Lewis structures used in organic chemistry do not correspond to the quantum mechanical model at all. This raises doubts whether assumption 1 can ever be validated using quantum mechanics.

Quantum mechanics certainly cannot validate assumption 1 directly. However, it can do so indirectly. If both models of explanation, quantum mechanics and organic chemistry, are applied to the same system, say, a reaction of a carboxylic acid and alcohol, then the outcome will be the same. Quantum mechanical calculation will show (at least in theory) that the most energetically favorable outcome of the reaction is to produce a carboxylic acid ester. A reaction mechanism with Lewis structures will also

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<sup>4</sup> A chemical bond achieved by sharing electron density between two atoms.

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arrive at the same conclusion using its conventions. Thus, assumption 1 is validated by quantum mechanics because its application to a system produces the same result as a quantum mechanical calculation. The prediction can also be validated experimentally by creating a reaction of two substances in a laboratory and characterizing the product using accepted spectroscopic and chemical techniques. The result will also agree with the prediction set forth by the two models.

Thus, assumptions used in organic chemistry explanations are derived and validated in the realm of quantum mechanics. However, the methods of this validation do not seem very clean-cut. The indirect, experimental method outlined above certainly does not follow the theoretical framework for reduction proposed by Nagel (Nagel 913). There are no laws in organic chemistry to describe the use of Lewis structures, and no suitable bridge principles can be formulated to connect Lewis structures to the quantum mechanical model. Hence, the use of Lewis structures, which are crude approximations of reality at best, has to be defended using an indirect argument of identical outcome whenever both organic chemistry and quantum mechanics are applied to a system.

The reason why assumption 1 can be validated is certainly not because organic chemistry reduces to quantum mechanics. Quantum mechanical explanation does not contain organic chemistry; if it did, Lewis structures could be perfectly reconciled with quantum mechanical models. Furthermore, there is a conflict of interests, problems, and methodology between organic chemistry and quantum mechanics that sets the two disciplines very far apart. Organic chemistry is purely qualitative. Its primary concern is to describe reactions, and its aim is more instrumental. Unlike quantum mechanics, it

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answers the question, “How do I synthesize x?”, but as a method of explanation of why the synthesis takes place the way it does, quantum mechanics provides stronger explanations. Hence, it brackets certain issues, like the ones listed as assumptions 1 and 2. This does not mean that organic chemistry is useless. Quite the contrary, it is tremendously useful for a laboratory scientist who wants to perform rapid syntheses with high product yield and high efficiency. If those are the goals of a chemist, using quantum mechanical models would be the long way around. Quantum mechanics, on the other hand, is quantitative. It makes use of complicated calculations and its aim is purely theoretical. It seeks to find the justification for reaction energetics. It is also more general than organic chemistry that concerns itself with specific reactions of specific compounds. Quantum mechanical problems deal with general rules of molecular behavior, and also, by virtue of being quantitative, quantum mechanics can generate law-like statements. Once molecular properties are described by mathematical equations, the explanation can become more deductive, and thus, quantum mechanics is more likely to make sweeping generalizations. Organic chemistry has no law-like statements, as its focus is on individual reactions. Viable research programs in organic chemistry often consist of finding and describing new useful reactions, but research programs in quantum mechanics are more concerned with advancement of the current theory. Organic chemistry has no overarching theory in the way quantum mechanics has. Generalizing about all possible chemical reactions is not the focus of organic chemistry, as it strives to describe particular reactions with as much detail as possible.

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Those considerations about the nature of organic chemistry and quantum mechanics are similar to descriptions of classical and molecular genetics Kitcher gives in “1953 and All That: A Tale of Two Sciences.” Kitcher argues that classical genetics does not reduce to molecular genetics because some explanations are more grounded in the classical model alone. He also opposes the view that our limited intellectual capabilities are the reason why molecular genetics does not seem to be explanatory of many cytological processes. The example of quantum mechanics and organic chemistry also serves to illustrate his point. Even if our knowledge of chemistry were so advanced to make organic chemistry quantitative the way quantum mechanics is, this would not change the fact that the purpose of organic chemistry is to explore particular reactions in detail, not create generalizations about all chemical reactions. Thus, there would still be a disconnect between quantum mechanics, which seeks a general theory of particle behavior, and organic chemistry, which explores reactions of carbon compounds in detail. Kitcher’s diagnosis of the failure of reductionism given in the second part of his paper also holds in this case. Kitcher says that the lack of law-like statements in classical genetics accounts for the failure of reductionism (Kitcher 980). More precisely, he argues that “lacking an account of theories which could readily be applied to the cases of classical genetics and molecular genetics, the attempt to chart the relations between these theories was doomed from the start” (Kitcher 980). Turning to the example at hand, organic chemistry lacks law-like statements. It is not concerned with proposing sweeping generalizations, so it is impossible to connect its principles to the principles of quantum

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mechanics by bridge laws. There is no set of laws to which such bridge principles could be applied.

Kitcher is concerned that arguing for autonomy of levels of explanation possibly carries metaphysical connotations. Yet, he does not address this concern explicitly. In fact, Kitcher's essay could be easily misread to argue that some kind of essence emerges on the cellular level that is not apparent on the molecular level. The case of autonomy of organic chemistry and quantum mechanics is perhaps easier to argue in purely physicalist terms. It cannot contain any elusive, metaphysical references to "life" the way biology can.

Justification for autonomy of the two levels of explanation can be found in Nancy Cartwright's view on the reality of physical laws. Cartwright argues that physical laws do not describe facts about reality (Cartwright 865). At best, they are approximations of how systems behave. Physical systems are subject to multiple effects at all times, and a composite of those effects cannot be simply treated as a result of an algebraic sum of laws that describe them.

Applying Nancy Cartwright's view of physical laws to the two models of description of molecular behavior, organic chemistry and quantum mechanics, it is apparent that neither of them states the facts. Organic chemistry is a symbolic system that approximates gross outcome of a chemical reaction, which, in reality, is a set of independent, simultaneous events convoluted together and taking place almost instantaneously (Cartwright 868). Quantum mechanics, with its generalizing objective, also does not describe behavior of a single molecule at any point during the reaction.

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Thus, both explanations are somewhat divorced from reality, and both describe small sections of a complicated process. Thus, it is possible to have two independent descriptions of the same physical system that tackle different problems and aspects and, in this respect, are autonomous. It is impossible, however, to hold this view and simultaneously believe that theories are real. Describing a chemical reaction as a gross effect of many instantaneous events, which can be only approximately described by a mechanism or a quantum mechanical model, calls for a specific kind of realism, which encompasses only entities. The reaction and its outcome is a real system, but theories that describe the system can be only approximate. Hacking asserts that it is possible to be anti-realist about theories, but realist about entities (Hacking 29).

Cartwright's example of multiple, joint processes leading to one outcome is a characterization of energy levels in a carbon atom (Cartwright 872). A similar example from the realm of organic chemistry and quantum mechanics is this reaction:



Organic chemistry makes a very convincing case for the mechanism of this reaction. The OH<sup>-</sup> ion displaces the bromine atom from the carbon chain. Experimental evidence suggests that the breaking of C-Br bond and attachment of the OH<sup>-</sup> happen simultaneously or almost simultaneously. To understand this reaction, no sophisticated

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knowledge of quantum mechanics is needed. In fact, reactions like these are part of every introductory organic chemistry curriculum.

Organic chemistry alone provides a detailed account of the effects of solvent composition and substrate concentrations on the outcome of this reaction. However, there is one element for which it cannot account. In the illustration, the bonds between C-Br in the substrate and C-OH in the product are shown according to three-dimensional stereochemical<sup>5</sup> convention. That is, the shaded triangular line between C-Br signifies that the bond is oriented away from the page, while the hatched triangular line between C-OH signifies that the bond is oriented into the page. In other words, there is an inversion of three-dimensional arrangement of the molecule during the reaction. This difference in geometry is a result of OH<sup>-</sup> attaching exactly 180° across from bromine atom. This effect, when described in terms of organic chemistry alone, seems very arbitrary. To fully explain the three dimensional geometry, shapes of molecular orbitals must be taken into account. In other words, there is a coherent reason for the inversion of three dimensional shape only from the quantum mechanical point of view.

As in Cartwright's example with carbon energy levels, here it is also apparent that theories are approximate. One theory cannot describe a complicated system alone, but when a composite of theories is used, inaccuracies will result because theories are rarely fully compatible with each other in the way Nagel's model of reduction postulates (Nagel 913). In the above example, using both organic chemistry and quantum mechanical

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<sup>5</sup> The symbolic representation pertains to three-dimensional arrangement of atoms in space, as explained in the text.

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models achieves the desired level of explanation, but the correspondence of Lewis structures depicted above to the elaborate quantum mechanical molecular orbital model is completely neglected. To achieve explanation, Lewis structures do not need to be directly translated to molecular orbitals using bridge laws. In fact, such translation would be hardly possible, as no suitable bridge laws exist. It is convenient to use Cartwright's approach and to assume that while the molecular entities exist, no theoretical model can describe them accurately. Because theoretical models do not exist, as opposed to molecular entities, no metaphysical thinking is needed to use two different and even contradictory models at the same time. When quantum mechanical explanation is used to account for the three dimensional geometry of a molecule, but explanation derived from organic chemistry is used to account for its chemical properties, no violation is committed. The real entity exists independently of the two explanations that can only approximate its real properties.

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