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Strategic Constraints on Interacting Fields: Quantum Chemistry and Organic Chemistry

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Abstract

The interaction between scientific fields may be subject to *strategic constraints*—that is, fruitful interaction between fields may require adapting one field to the strategies informing the other. One way the concepts within an interfield field develop is by recrafting concepts originating in one practice in terms compatible with the strategies guiding the other. This conceptual accommodation may be a prerequisite to fruitful interactions between fields with different central problems. I explore these themes by considering the *strategic constraints* operative in the interfield field of quantum chemistry and the conceptual accommodation required for application to organic chemistry.

Introduction

Lots of terms have been introduced to allow philosophers to talk about units of concerted scientific activity: disciplines, practices, communities sharing a paradigm, etc. I am going to use Darden and Maull's concept of a "field" because it emphasizes some aspects of the consensus guiding concerted scientific activity that are important for my purposes in this paper. According to Darden and Maull, a field consists of: a central problem, a domain of items related to that problem, a strategy for solving the problem, techniques for implementing that strategy, and a theoretical apparatus (laws, theories, or concepts) that support that strategy (Darden and Maull 1977, 44). It is plausible, I hope, to think about both organic chemistry and quantum chemistry as fields in this sense, though by doing so one necessarily underrepresents the full range of these immense regions of scientific activity.

For organic chemistry, the, or at least a, central problem is novel synthesis, which requires developing the manipulation and control of organic transformations required in such a synthesis. The domain is the chemical space of actual and potential organic molecules individuated by their *bond structures.* The techniques for solving synthesis problems include functional group classification, catalogs of reaction types, reaction mechanisms, retrosynthetic analysis, etc. The theoretical apparatus that supports the manipulation and control of organic reactions is vast, but would certainly include things like valence-bond theory, molecular orbital theory, orbital diagrams, theories of

resonance, transition-state theory, etc. The strategy that guides organic chemistry in the solution of novel synthesis problems isn't often made explicit and will receive more detailed exposition throughout the course of the paper. For the moment I will just give it a name: a substructural, compositional strategy. This means, to a first approximation, that organic chemists understand novel molecules as being composed out of substructural components whose chemical behavior can be understood because they occur in other, simpler molecules or reactions that have already been investigated.

For quantum chemistry, on the other hand, the central problem is the approximate solution of the time-independent Schrödinger equation under the fixed-nuclei approximation. The domain is the space of geometrical arrangements of fixed nuclei (or *geometrical structures*; see Hendry (2016) for an account of the different senses of *structure*) with particular numbers of electrons. The strategies for solving this problem include perturbation theory and the variational technique, where trial wavefunctions are proposed and evaluated by their ground-state energy. The techniques for implementing these strategies include the valence-bond and the molecular orbital approaches, configuration interaction, and density-functional theory (which skips the wavefunction and directly computes energy). The theoretical apparatus that supports this strategy and these techniques includes the Schrödinger equation along with justifications of various approximation techniques. Quantum chemistry, when it is understood this way, is itself an *interfield field* (and not just an interfield theory)—it is a field that "functions to make explicit and explain relations between fields" (Darden and Maull 1977, 48), in this case quantum mechanics and chemistry. It does this, in part, by borrowing the concept of a *geometrical structure* and then imposing this on the mathematical framework of quantum mechanics by way of the fixed-nuclei approximation. It is not, then, a field that should be understood as aiming to "reduce" chemical phenomena to quantum mechanics, rather it is a field that strives to make quantum mechanics relevant in a context where the geometrical structure of molecules is an established and ongoing concern. It is a field, not a theory, because there are lots of distinct strategies and techniques for solving this central problem in a way that makes it relevant to chemists.

The focus of this paper, however, is not on the relationship of quantum chemistry to quantum mechanics, but rather on the relationship between quantum chemistry and organic chemistry. The cognitive tools used by organic chemists have developed, for at least the last 90 years, in interaction with the work of quantum chemists. In many cases, quantum chemists have ended up supplying rationalizations, or articulations, of ideas that had already begun developing independently in the work of organic chemists (Coulson 1955, Harris 2008). Classic examples here would include the quantum mechanical reinterpretations of the covalent bond, or of mesomerism between valence-bond structures. In other cases, such as the Woodward–Hoffman rules, novel theoretical principles of practical import have emerged out of this interaction. There can be little doubt that these sorts of developments have had a profound impact on the "theory" of organic chemistry, and thus on the ways that such chemists explain, predict, and design chemical reactions (Wilson 1976). Still, these sorts of contributions are fundamentally integrations of chemical and quantum chemical ideas in that they begin with a perspective on molecules that is crucial to organic chemistry and then seek to refine it with ideas from quantum chemistry.

They are not attempts to replace or supplant the cognitive tools and strategies developed by organic chemists; rather, they integrate quantum chemistry with this pre-existing approach (Gavroglu and Simões 2016, Woody 2012). In this paper, I try to develop an account of why this is the case. The basic idea is that the tools and strategies have been crafted (at least in substantial part) to solve a particular sort of problem—the synthesis of novel molecules—which requires tracking patterns in chemical behavior that are not necessarily captured from a purely quantum chemical perspective. By focusing on what is required in order for solutions of the central problem of quantum chemistry to be made relevant to solutions of the central problem of organic chemistry, it is possible to specify the *strategic constraints* under which these two fields interact. Just as *geometrical structure* needed to be imposed on the pure formalism of quantum mechanics in order to create the central problems of the field of quantum chemistry, so I will argue that something much like *bond structure* (in that it is compatible with a substructural, compositional strategy) must constrain the solutions to the central problems of quantum chemistry, if they are to be explanatorily useful in solving the central problems of organic chemistry.

Trade-offs in quantum chemical explanation

At first pass, one might think that the limitations on the applications of quantum chemistry to organic chemistry are purely pragmatic; that the only constraints on the use of quantum chemistry in contributing to the solving of synthesis problems are computational, a consequence of the large size of many of the organic molecules with which synthetic chemists are concerned. However, as many quantum chemists, as well as historians and philosophers of chemistry, have pointed out, there is a trade-off at play between the predictions and explanations that quantum chemists can supply in support of organic chemistry (Coulson 1960, Primas 1975, Woody 2000, Hettema 2017). Even when a sophisticated quantum chemical treatment of a particular molecule is available, and accurate predictions are possible, it does not follow that explanations useful to the synthetic chemists can be produced from this treatment. The techniques for solving the central problem of quantum chemistry that are well suited to precise prediction are not necessarily well suited to generating useful explanations in organic chemistry, and vice versa. It has been tempting for some to regard these trade-offs as the consequence of epistemic opacity, thereby assimilating quantum chemistry to other cases, such as simulation modelling, where there are similar trade-offs between prediction and explanation (Lenhard, 2014).

I think it is more useful to understand the case of quantum chemistry and its trade-offs between prediction and explanation as resulting from the "universal" character of the chemical behavior of interest to organic chemists. I am here using "universal" in the sense articulated by Batterman (2002, 13) while changing his talk of "systems" into talk of "molecules." Chemical behavior is universal in this sense, when:

- the details of the molecule (the complete bond and geometrical structure of the molecule) are largely irrelevant for describing the behavior of interest;
- many different molecules with completely different structural details will exhibit identical behavior.

One obvious example of the "universal" behavior of molecules of interest to organic chemists can be seen in the functional group classification of a molecule, which is so central to how organic chemists think that it is the foundation of organic nomenclature. When an organic chemist describes something as a "carboxylic acid," this conveys a tremendous amount of information about the behavior of the molecule, including chemical and physical properties, as well as reactive behavior. Furthermore, this behavior is presumptively shared with a vast and indeterminate number of other molecules which differ from the named molecule in their bond and/or geometrical structure. In other words, being a carboxylic acid, and demonstrating the behavioral patterns associated with this classification, is a universal property of molecules (as individuated by their bond structure, or, doubly so, by geometrical structure). It is a universal property that can be ascribed to a molecule on the basis of a substructural component of its full bond structure: for any R, if a molecule can be written as RCOOH then it is a carboxylic acid. Almost all organic chemical taxonomy is universal in this way: it is meant to characterize similarities in chemical behavior across a range of different bond and/or geometrical structures, and the behavior is linked to, or originates in, some substructural component of the molecules that demonstrate it.

Batterman also usefully distinguishes two distinct why-questions that might be asked about the universal behavior of a particular system. Roughly speaking, we might be asking for an explanation of the behavior of the particular, or we might be asking for an explanation of the pattern of universal behavior; he calls these type (i) and type (ii) explanations, respectively. Returning to our carboxylic acid example, one might ask a type (i) question like "Why is the K_a of acetic acid 1.76×10^{-5}?" or one might ask for an explanation of a pattern of behavior, like "Why are carboxylic acids more acidic that alcohols?" Often, in organic chemistry, one addresses the request for an explanation of a pattern by considering a particular case. For instance, one might address the question of the difference in the acidity of carboxylic acids and alcohols by comparing the acidity of acetic acid to that of ethanol. If one were to pursue this strategy of explaining the general pattern by considering the particular case, it would not suffice to simply produce two type (i) explanations of the K_as of acetic acid and ethanol and then to show that one is larger than the other. Instead, one would have to show that the difference in acidity issues from the features of acetic acid and ethanol that make them representatives of the larger classes for which they stand, namely carboxylic acids and alcohols. Since, as I indicated above, most chemical taxonomy is based on substructures, explanations of patterns in chemical behavior must appeal to the substructures that make particular molecules representative of the relevant chemical taxon. And indeed, in this particular example, the explanation is in terms of the resonance stabilization of the carboxylate ion relative to the carboxylic acid (while there is no such stabilization difference in the alcohol), and it doesn't depend on the rest of the chemical structure. The same argument would apply, therefore, for any other pair of carboxylic acid and related alcohol. In this way, an explanation of the behavior of a particular molecule (or a particular pair of molecules, as in the example above) can be used to explain a pattern of behavior, but only by restricting that explanation to features that that particular shares with other members of the class it is intended to represent.

So now we can return to the question of trade-offs between explanation and prediction in quantum chemistry. The basic idea is that applications of quantum

chemistry that are good for answering type (i) why-questions are, as a consequence, not generally good for answering type (ii) why-questions, and vice versa. To see why this is so, it is useful to compare what is required in order to give an accurate prediction or explanation of the properties of an individual to what is required to explain the properties of an individual as a representative of a chemical taxon. In the first place, type (i) explanations of the properties of a particular generally aspire to as much numerical precision as possible—the more accurately you can reproduce experimental values, the better testament to the power of quantum chemistry. Type (ii) explanations, on the other hand, are more often after qualitative, contrastive, or relative properties. These sorts of properties are the sorts of properties that can be shared by broad classes of structurally diverse molecules, and which can thereby figure in the universal behavior that characterizes that class. Carboxylic acids may all be acidic and more acidic than corresponding alcohols, but they do not all have the same K_a. Explaining why acetic acid has the precise K_a that it does requires distinguishing it from other carboxylic acids, and thus taking account of all of the features make it different from the other molecules in its same taxon. Explaining why acetic acid is more acidic than ethanol in order to explain a general pattern in the behavior of carboxylic acids requires, on the other hand, *not* appealing to any features of acetic acid that distinguish it from other carboxylic acids.

In order to explain the behavior of a molecule in terms of substructures of that molecule that occur in other members of the same chemical taxon (and thus to provide type (ii) explanations), the behavior of whole molecules must be explicable in terms of the behavior of their substructures. Or to give it a name, chemical behavior must be understood compositionally. Furthermore, the substructures out of which such a representative is understood to be composed must be capable of recurring in other structures. This is what makes the explanation generalizable. Traditionally, the various types of chemical bonds have been the fundamental units of chemical compositionality: they are the fundamental recurring structural subunits out of which the behavior of organic molecules is compositionally understood. For instance, carbon–hydrogen bonds are substructural components of most organic molecules, and they behave similarly in all these different structural contexts. These, along with the other types of bonds, are the most basic components of our descriptions of organic molecules, and the complete bond structure is what organic chemists use to individuate chemical types. Substructures can recur in molecules insofar as they share a bonding pattern, and these shared substructures underwrite the idea that two molecules are structurally similar in some way, and thus provide the potential for type (ii) explanations. Bond structure thus supports the substructural compositional strategy behind organic chemists' attempts to provide type (ii) explanations of chemical behavior; furthermore, it underwrites the whole taxonomic framework that organic chemists use to make sense of their domain.

Unfortunately, but perhaps not surprisingly, the "bonds" that play such a fundamental role underwriting the taxonomy central to organic chemistry are not essential features of attempts to solve the central problem of quantum chemistry. In fact, it is generally the case that attempts to get accurate type (i) explanations or predictions of properties of molecules require abandoning the sorts of strategies and approximations that are straightforwardly interpretable in terms of chemical bonds, which serve as a foundation for structural similarity. The strategies and

approximations compatible with a standard two-atom bonds are "localization" strategies that effectively ignore or cordon off the effects of delocalized electrons. If you are after accuracy, then localization is the enemy because it introduces unnecessary approximations which limit how close one can get to the "actual" wavefunction, and thus to accurate numerical values of chemical properties. To be accurate, the whole must be recognized to be more than the sum of its pairwise parts, but to be generalizable, properties of that whole must be understood to issue from parts that can recur in other cases. Or to put it another way, in order to rationalize universal patterns in chemical behavior, you need to think of molecules as approximate sums of their recurrent parts, but if you think of them as approximate sums of recurrent parts you can't calculate very accurate values for their individual chemical properties. Thus, the trade-offs between prediction and explanation that many have noticed in quantum chemistry are the consequence of quantum chemists attempting to answer two different sorts of why-questions. Cutting edge, computation-intensive work is useful for answering type (i) why-questions, while other strategies are required if quantum chemistry is to address type (ii) why-questions. Different strategies are required because organic molecules simply aren't sums of their pairwise parts, but rationalizing patterns in their chemical behavior and properties requires thinking of them as such.

If this is right, then I hope to have explained the source of the competing demands on quantum chemistry that result in trade-offs between explanation and prediction, but what I haven't yet done is to explain why organic chemists think of molecules the way that they do. By returning to the central problem which I characterized in assimilating organic chemistry to Darden and Maull's conception of a field, it is possible, I think, to understand why organic chemists insist on understanding the behavior of molecules in terms of structural subcomponents. This way of thinking reflects the strategy chosen for solving their central problem, which is roughly the synthesis of novel compounds. And, thus, in order for quantum chemistry to contribute explanations that support the strategy used in organic chemistry, the approaches taken in quantum chemistry must be compatible with a substructural compositional strategy; that is, they are subject to strategic constraints originating in organic chemistry.

Solving the central problem of organic chemistry

Not surprisingly, chemists who are interested in crafting novel syntheses describe and categorize the compounds they encounter in ways that help to anticipate the chemical reactions in which those compounds might be involved—their classification systems are outward looking. More specifically, the bonds, structural formulas, and functional groups which are the core classificatory tools of the organic chemist are, in substantial part, intended to capture a notion of structural similarity which in turn situates organic compounds within a space of possible chemical transformations. The strategy by which synthetic chemists achieve this outward-looking classificatory practice is compositional. By this I just mean that the reactive behavior of an organic compound is approached or approximated as a composition of the behavior of its recurrent parts. These parts are in turn supposed to behave in similar ways whenever they recur in organic compounds. This strategy is dictated by the fact that synthetic

chemists must anticipate the behavior of novel compounds. If a compound has never been made or interacted with before, there is no databank of known reactions that apply to it directly. Instead, in order to get a handle on how the novel compound will, or might, behave, it is necessary to identify similarities between its structure and the structures of compounds whose behavior is known. This is done by identifying substructures of the compound of interest whose behavior has been investigated (and which is presumed to be similar in the novel circumstances).

While the bond and functional group composition of a novel molecule does provide initial guidance as to the reactions in which the compound might be involved, the synthetic plausibility and usefulness of these reactions often depends on the structural details of the novel molecule. To anticipate, insofar as it is possible, the synthetic impact of those details, the chemist will make use of the mechanisms of the potential transformations. These mechanisms indicate what kinds of other structural features will influence the reaction outcomes or plausibility in particular structural environments. By analyzing the structure of the novel compound, the chemist can then identify which of those particular features are present, and then make a much more refined prediction about the plausibility and usefulness of a potential transformation. By understanding the mechanisms of transformations, the organic chemist is thereby able to correct, or refine, the compositional strategy for anticipating novel behavior, and this sort of mechanistic refinement has allowed for much more sophisticated syntheses. Even with this sort of refinement, however, it is generally only possible to provide qualitative or contrastive predictions of how a novel compound will behave. Still, these limited sorts of anticipations of the behavior of novel compounds have turned out to be enough to support the seemingly unlimited capacity of organic chemists to produce novel syntheses of compounds of interest. So, getting a handle on chemical behavior for the purposes of novel synthesis involves disassembling organic compounds into their reactively significant parts and then piecing those parts back together, with appropriate corrections, to understand the behavior of novel molecules. This strategy has been immensely successful.

Because the strategy for solving the central problem of organic chemistry demands that the cognitive tools of the organic chemist are outward-looking and compositional but doesn't require quantitative precision, there is good reason for the organic chemist to prefer imprecise explanations of a pattern to precise, particular predictions. As a result, many of the applications of quantum chemistry in organic chemistry accommodate the strategic demands of organic chemistry by using concepts or approaches to the approximate solution of the time-independent Schrödinger equation that are compatible with a substructural, compositional strategy. This conceptual accommodation often takes the form of using approximation schemes, such as valence-bond or molecular orbital approaches, that can reintroduce compositionality, and thus structural similarity, by creating wavefunctions in a systematic way from recurring and separable pieces. In such approximation schemes, it makes sense to say, for instance, that all carbon–carbon double bonds are formed by overlap of the same types of atomic orbitals. Then, even if other aspects of the system are different, there will be a component of the wavefunctions of two distinct alkenes that is the same (or approximately so), and so some results applicable to one case might also apply to the other. In this way, quantum chemistry can contribute explanations of the sorts of universal behavior

that are useful in anticipating the reactive behavior of novel molecules. The potential for type (ii) explanations is generated by composing the wavefunctions of complex systems out of standard parts, which then behave the same way across a range of structures and can therefore possibly explain a pattern in behavior. Of course, the cost of thinking of wavefunctions as built out of separable, standard parts that recur across a range of structures is that the true wavefunction cannot be approximated as accurately using these limited components. This means that different approaches to solving the central problem of quantum chemistry must be taken when type (i) explanations, or precise predictions, are desired.

Conclusions

As historians and quantum chemists themselves have noted,[1] large parts of quantum chemistry (and in particular those parts most useful to the organic chemist) have emerged from the reciprocal interaction of chemistry and quantum mechanics. This reciprocal interaction has led to important developments in the theory of organic chemistry, but it has often done so by making approximations or assumptions motivated, at least in part, by their capacity to accommodate the pre-existing concepts and strategies of organic chemistry.[2] Thus, quantum chemistry, insofar as it unifies quantum mechanics and chemistry, often does so by finding ways to recast or assimilate concepts from one field in terms amenable to application in another. In the useful terms of Woody (2012), the concepts of quantum chemistry are an amalgamation of concepts from quantum theory, classical structure theory, and mathematical approximation techniques. What this paper adds to this now—hopefully—increasingly familiar conception of quantum chemistry is an explanation of why quantum chemistry has to make these sorts conceptual accommodations in order to be useful to chemists, particularly synthetic organic chemists. I tried to show that the classificatory apparatus of chemistry reflects a particular strategy, and operates at a level of generality, that suits it to the interests of synthetic chemistry. The core technology of quantum chemistry does not, by itself, operate at the appropriate level of generality or in a form that is compatible with this strategy. Thus, the fruitful contribution of quantum chemistry to organic theory required the development of approximation schemes, what I referred to above as "localizing assumptions," that implemented the core technology of quantum chemistry in a way that is compatible with this strategy.

Woody (2000, 2012) describes how spatial representations such as orbital diagrams allow for quantum chemical explanations of classes of chemical facts, thereby "bridging the gap between quantum theory and chemical practice." She even invokes quantum chemical explanations of this sort to suggest that "requirements for satisfactory explanation are importantly discipline specific and dependent on the overarching aims and practices of given scientific communities" (2012, 461). Likewise, Coulson (1960, 173) describes how satisfactory explanations in chemistry must be

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[1] Gavroglu and Simões (2016) and Harris (2008) are historians that make this sort of claim, while for quantum chemists Coulson (1955) and Wilson (1976) are good examples.

[2] Sutcliffe and Woolley (2012) develop this point about geometrical structure, while Coulson (1961) makes it for bond structure.

given in terms of concepts that are "adequate or suitable" rather than merely reporting the numerical results of quantum chemical calculations. What this paper has added to these insights is an explicit account of the constraints put on the explanatory concepts of organic chemistry by the aims that have shaped the field. It is because of the guiding interest in synthesis, I have argued, that the explanatory concepts of organic chemistry must support a compositional strategy; this is how they manage to be outward looking and thereby support the reasoning by structural analogy crucial to crafting plausible syntheses of novel compounds. If this is right, then what makes a concept or classification "adequate or suitable" for use in organic chemistry is its compatibility with the compositional strategy adopted by the discipline. Woody's orbital diagrams are one way to reframe quantum chemistry so that its explanations are compositional in the appropriate sense, and this explains, from my point of view, why they have been such a useful tool for organic chemists. However, there are other ways of ensuring compatibility with compositionality that do not rely on diagrams or spatial representations, for instance the "localizing assumptions" described by Coulson. Thus, I hope that identifying compatibility with a substructural, compositional strategy as the key feature of the explanatory concepts in organic chemistry will allow for a broader, and principled, understanding of the sorts of conceptual accommodation required to bridge the gap between quantum chemistry and chemical practice.

Most generally, I hope to have shown that the interaction of scientific fields can be subject to *strategic constraints*—fruitful interaction between fields may require finding ways to adapt the techniques and concepts involved in one field to the strategies guiding the other. In the case of organic chemistry, the strategy that is enlisted in solving its central problem(s) requires a classificatory and explanatory scheme that allows the behavior of complex molecules to be understood in terms of recurring substructural components. Bond structures and chemical taxonomy developed in response to this demand, but quantum chemists had to find ways to recreate this compositionality within their own framework in order to generate the sorts of explanations that are useful in solving the central problem(s) of organic chemistry. By thinking of the interaction of these two fields in terms of their central problems and guiding strategies, it was possible to explain both important historical features of their co-development and to provide a general and principled account of the sorts of conceptual accommodation required for their successful integration. This provides a more fruitful approach to thinking about the important ways that scientific fields interact than does a more standard reductionist framework.

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