

The Physicists, the Chemists, and the Pragmatics of Explanation

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In this paper I investigate two views of theoretical explanation in quantum chemistry, advocated by John Clarke Slater and Charles Coulson. Slater argued for quantum-mechanical rigor, and the primacy of fundamental principles in models of chemical bonding. Coulson emphasized systematic explanatory power within chemistry, and continuity with existing chemical explanations. I relate these views to the epistemic contexts of their disciplines.

1. Introduction. In 1929, not long after the birth of quantum mechanics, P. A. M. Dirac claimed confidently that

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation. (1929, 714)

Now Dirac's call can be answered with different kinds of activity. On the one hand, the problem situation—the intractability of exact quantum mechanics—suggests that the novelty he mentions will be mathematical, teasing out structure that is in some sense “already there” in the exact equations. On the other hand, the phrase “approximate methods of *applying* quantum mechanics” might suggest some *descriptive* novelty. The “whole of chemistry,” of course, includes polyatomic molecules, which present a new order of complexity. Perhaps new, more tractable kinds of

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[‡]Research towards this paper, and my attendance at the PSA meeting were supported financially by the Leverhulme Trust and the British Academy.

Philosophy of Science, 71 (December 2004) pp. 1048–1059. 0031-8248/2004/7105-0035\$10.00
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model will be required to understand the behavior of polyatomic molecules, not directly related to the successful treatments of the hydrogen atom. Views on which of these two approaches should be taken by the new discipline of quantum chemistry did not divide along disciplinary lines. Nevertheless, I call them the views from physics and chemistry respectively, for the issue is one of autonomy and authority. Should molecular quantum mechanics be regarded as a descriptively complete import from physics? Or may quantum mechanics be adapted as required to the explanatory demands of chemistry? In what follows I will attempt to fill out the details of these two positions through the methodological reflections of John Clarke Slater and Charles Coulson.

In fact, the early 1930s brought *two* approximation schemes that promised workable results for molecules. Both were based on approximations conceived in Europe in the late 1920s, and elaborated in the US in the 1930s. The Heitler-London-Pauling-Slater valence-bond method modeled wavefunctions for molecules as superpositions of states corresponding to classically bonded structures. The resulting quantum-mechanical states were 'resonance hybrids' of the canonical structures from which they were formed. The Hund-Mulliken molecular-orbital approach built up delocalized molecular orbitals from available atomic orbitals. The ensuing debate between defenders of the two schemes complicates and enriches discussion of the above issue, for it also occasioned frequent appeal to general epistemic principles and values.

2. The View from Physics: Slater. It is perhaps natural for theoretical physicists to see the application of physical theories to chemical systems as an imperialist process in which a lawless domain that borders physics is brought to order: so natural in fact, that the hubris of some physicists predated the emergence of quantum mechanics. In a presentation of 'old' quantum-theoretic atomic models published well before the advent of quantum mechanics, Max Born commented that

When we contemplate the path by which we have come we realize that we have not penetrated far into the vast territory of chemistry; yet we have travelled far enough to see before us in the distance the passes which must be traversed before physics can impose her laws upon her sister science. (Born, quoted in Nye 1993, 229)

Now it would be natural to expect those who played only a distant part in the development of quantum chemistry to take a loftily ambitious view of what quantum mechanics could explain in chemistry. But John Clarke Slater, one of the architects of the valence-bond approach, was similarly convinced of the primacy of fundamental physical principles.

After completing a Ph.D. at Harvard under P. W. Bridgman, Slater

worked with Bohr in Copenhagen in the academic year 1923–1924 (Hoddeson 1990). On his return from Europe, Slater made, during the late 1920s and early 1930s, a slew of important contributions to the quantum mechanical theory of many-electron systems, and of molecular structure and bonding (Park 2000). Although they constructed the same model of directed valence, Slater's style and motivation were quite different from Linus Pauling's. Buhm Soon Park argues that Slater's papers on hybridisation were an attempt to "lay out the procedure for solving the Schrödinger equation for molecules in general, rather than carry out computations for actual examples" (Park 2000, 461). Moreover, Slater sought general theoretical justification for his approximations, rather than computational tractability and physical plausibility in the case at hand.

Philosophically, Slater followed Bridgman's pragmatism, and was consequently uninterested in, even hostile to, discussion of the interpretation of quantum mechanics: like other American scientists of the time, he preferred to get on with applying the theory (Cartwright 1987; Schweber 1990, section 4). In some tension with this pragmatism, however, were the reductionist philosophical views he also professed, and the methodological outlook they inspired. As early as 1933, Slater complained, "The study of molecular structure has been too much based on particular models, rather than on general principles" (quoted in Schweber 1990, 396), the 'principles' being physical ones. Moreover, as he argued in an undelivered lecture written in 1937, physics is

. . . the simplest science, and the one which most nearly gets us back to first causes. Its laws . . . its fundamental particles, seem as basic in the scheme of things as scientists have succeeded in getting. Next, now hardly distinguishable from it, comes chemistry. (Slater, quoted in Schweber 1990, 391)

Slater's views on the valence-bond and molecular-orbital approaches are revealing. While the chemists argued over the relative merits of the valence-bond and molecular-orbital theories, and sought to defend and extend their explanatory uses, in his textbook *An Introduction to Chemical Physics* (1939), Slater presented them as two approximation methods, differing "not in their fundamentals, but in the precise nature of the analytical steps used" (1939, 368). A proper understanding of the forces between atoms and molecules, he thought, should appeal to "fundamental principles, without reference to exact [for which read, particular] methods of calculation" (368). Slater's ecumenism on the issue of valence-bond versus molecular-orbital theories looks to be a further expression of his reductionism. The two schemes should, in his view, be regarded not as competing explanations of molecular bonding, but as logically (though not practically) dispensable aids to understanding the content of quantum

mechanics with regard to the behaviour of molecules (see also Gavroglu and Simoes 2000, 427–431).

Slater saw himself as an upholder of standards of rigour that were transgressed by others engaged in applying quantum mechanics to molecules. In 1950 he complained that

[T]he theory of chemical valence was taken up by the chemists, who rather naturally did not have enough fundamental insight into the nature of wave mechanics to make the contributions to the theory which were really needed to put it in a satisfactory form, but instead proceeded on the one hand to a great extension of its mathematical formalism, on the other to stretching the theory far beyond what was justified by its crude nature in making comparisons with experiment, with the result that most of the results obtained by the chemists since that time are suspect by the physicists. (Slater, quoted in Schweber 1990, 389–390)

Towards the end of his life, he set out his own positive views on what these standards should be:

I was never satisfied with any theory that didn't come out of the fundamental principles of quantum mechanics perfectly straight forwardly, and I still stick to that point of view. Whereas a great many people were willing to make what they would call models—put in something that would look plausible, out of which you could get formulas that would describe the facts, but where you could not derive this model from fundamental theory—I felt here we had a fundamental theory and a challenge to be able to explain everything we see around us in terms of that fundamental theory. So I have always discarded anything that didn't fit into that. (Slater, quoted in Schweber 1990, 396)

Slater presents a consistent normative view of approximate theorizing, which I will try to flesh out in the rest of the section. The starting point is that quantum-mechanical explanation should be a subsumptive process, in which laws, facts and tendencies associated with molecular structure and bonding are shown to be special cases of the quantum mechanics of systems of charged masses. The 'fundamental principles' of quantum mechanics, plus the special assumptions and constants required for its application to systems of charged particles, are sufficient to determine a canonical quantum-mechanical treatment for any atom or molecule. The explanatory content of the theory with respect to particular molecules is delimited precisely by this 'exact' treatment.

Of course, the intractability of quantum-mechanical equations renders this explanatory content inscrutable, but the ideal of subsumptive expla-

nation can be upheld even in idealized and approximate treatments, so long as there is warranted satisfaction that whatever is explained using an idealized or approximate quantum-mechanical equation could also be explained using the exact treatment, supposing that it were tractable. In short, approximate or idealized ‘model’ treatments are legitimate in so far as they are proxies for exact ones. That failure of autonomy restricts their proper uses. Firstly, a feature of the model’s structure can legitimately be appealed to in explanation only if it is shared by the exact treatment. Hence the approximate or idealized model should have a clear mathematical relationship to the exact treatment: if the empirical value of some molecular quantity is compared to one calculated from a model treatment, we need to know that the model calculation gives us something close to the ‘exact’ value. Second, where a model treatment is based on approximations or idealizing assumptions, conclusions derived in the model apply only where those assumptions hold. Lastly, features of an approximate model that will disappear when the limit of the exact equations is approached (and so are not shared by the exact treatment) can have no place in explanation (see also Hendry 1998, section 2). Slater’s even-handedness with respect to the valence-bond and molecular-orbital approaches follows immediately: since the two methods converge as they approach the exact limit, they should be ignored where they diverge.

3. The View from Chemistry: Coulson. Charles Coulson was the first Cambridge research student of J. E. Lennard-Jones, who was the first occupant of the first Chair in Theoretical Chemistry in the UK. After receiving his Ph.D. in 1936 for a thesis covering the electronic structures of H_3^+ and methane, a Prize Fellowship at Trinity College allowed Coulson time to pursue a molecular-orbital treatment of fractional bond orders in arenes and conjugated polyenes, complementing a valence-bond treatment published by Linus Pauling and others in 1935. A subsequent senior lectureship at Dundee lasted through most of the war (Coulson was a conscientious objector), after which he was appointed to a fellowship at the Physical Chemistry Laboratory in Oxford, and then a chair in theoretical physics at King’s College London, in 1947 (Altmann and Bowen 1974). His prominence was secured in 1952, with his appointment as Rouse Ball Professor of Mathematics at Oxford, and the first edition of his influential textbook *Valence*.

Valence promoted the molecular orbital approach, displaying its explanatory wares, especially within organic chemistry where valence-bond theory had hitherto been regarded as more successful. Coulson was generally even-handed in the book, however. He included chapters on the valence-bond method, whereas Pauling had not done the same for molecular-orbital theory in his textbook *The Nature of the Chemical Bond*.

He also incorporated comments from Pauling into the second and later editions (see Gavroglu and Simoes 2000, 442–444). Like Slater, he included comparisons of the two methods (Coulson 1961, 146–161 and 274–275), noting that in fully sophisticated applications of the two methods, they approached equivalence. Unlike Slater, his ecumenism did not undermine the explanatory autonomy of the two schemes. Both, he admitted, introduced gross approximations, compounded by “limitations in the amount of calculation that is worth while”, and so their value lay in “qualitative understanding, and not quantitative calculation” (1961, 146). Despite their equivalence in the limit of fully sophisticated calculations, the tractability and usefulness of their applications, and the qualitative understanding they afforded would frequently diverge. (For a more direct relationship between qualitative understanding and idealization see Weisberg 2004.) But “where both theories predict similar conclusions, there is considerable ground for believing that these conclusions are correct” (1961, 158).

At the beginning of his presentation of the valence-bond methods in chapter five of the book he remarks:

It is not unfair to say that . . . in practically the whole of theoretical chemistry, the form in which the mathematics is cast is suggested, almost inevitably, by experimental results. This is not surprising when we recognize how impossible is any exact solution of the wave equation for a molecule. Our approximations to an exact solution ought to reflect the ideas, intuitions and conclusions of the experimental chemist. (Coulson 1961, 113–114)

By “experimental results” Coulson means experimentally calibrated theoretical constants associated with molecular structure: the turbulent history of molecular structure in the nineteenth century surely qualifies as ‘theoretical’ any experimental results presented in terms that presuppose it. In comparing the valence-bond and molecular-orbital treatments of bond polarity, he argues that although the molecular orbital presentation is “more natural and conceptually the simpler,” “the structures used in the v.b. description do correspond to pictures long familiar, in classical form, to experimental chemistry.” Moreover, “this link with the older and more conventional language is of considerable value” (1961, 154).

Contrast Coulson’s remarks about approximations “reflecting the ideas, intuitions and conclusions of the experimental chemist” with the caution one finds in the “view from physics” about misinterpreting arbitrary elements of a scheme of approximation. In the “view from physics” the explanatory power of a model treatment should depend on some aspect of its mathematical form only where this is shared by the exact treatment. In chapter 9 of *Valence*, Coulson compares valence-bond and molecular-orbital treatments of conjugated polyenes and arenes. He concludes that

although they are far from quantitatively reliable, they provide “general outlines” which

enable us to understand a very large part of the field of organic chemistry, and to organize it and correlate its different sections: they provide us with at very least a qualitative understanding of the essential processes at work. Taken as a whole, both the v.b. and m.o. approximations seem about equally good; and any theoretical conclusion cannot be regarded as substantiated unless it is predicted by both. (Coulson 1961, 275)

Slater demands that a quantum mechanical theory of molecules “come out of the fundamental principles of quantum mechanics perfectly straight forwardly.” Coulson requires rather that results for molecules within either the valence-bond or molecular-orbital approaches be corroborated by corresponding results within the other framework. (This may seem to rule out the two approaches being explanatorily non-equivalent, but remember that Coulson thinks that their explanatory power lay in *how*, in qualitative terms, they achieve the numerical results they do, which typically diverge even if the results do not.) On one measure, Coulson’s requirements of approximate models seem weaker than Slater’s, but notice that he adds a desideratum that is *independent* of physics: explanatory and predictive efficacy in systematizing existing chemical theory.

At a conference on molecular quantum mechanics in Boulder, Colorado in 1960, Coulson commented in an after-dinner speech on the trends he had discerned in the conference papers (see Coulson 1960). Computational quantum chemistry, he noted, was thought by some quantum chemists to be “so remote from the normal natural conventional concepts of chemistry, such as bonds, orbitals, and overlapping hybrids, as to carry the work itself out of the sphere of real quantum chemistry” (1960, 172). Foreseeable electronic computers offered “effectively exact” solutions to the Schrödinger equation, but although *ab initio* approaches were ostensibly more accurate, they faced a practical limit of about 20 electrons, and were difficult to interpret in terms of traditional chemical concepts. For chemists working on the ‘posterior’ approaches,

[t]he role of quantum chemistry is to understand these concepts and show what are the essential features in chemical behavior. These people are anxious to be told why, when one vinyl group is added to a conjugated chain, the uv absorption usually shifts to the red; they are not concerned with calculating this shift to the nearest angstrom; all they want is that it should be possible to calculate the shift sufficiently accurately that they can be sure that they really do possess the fundamental reason for the shift. Or, to take another example,

they want to know why the HF bond is so strong, when the FF bond is so weak. They are content to let spectroscopists or physical chemists make the measurements; they expect from the quantum mechanician that he will explain *why* the difference exists. But any explanation *why* must be given in terms which are regarded as adequate or suitable. So the explanation must not be that the computer shows that $D(\text{H}-\text{F}) \gg D(\text{F}-\text{F})$, since this is not an explanation at all, but merely a confirmation of experiment. Any acceptable explanation must be in terms of repulsions between nonbonding electrons, dispersion forces between the atomic cores, hybridization and ionic character. (Coulson 1960, 173)

Now Coulson was a scion of Cambridge mathematics, confident of the central role of advanced mathematical tools in solving chemical problems, and many of his efforts certainly were directed towards developing mathematical methods for quantum chemistry (Altmann and Bowen 1974, 107–110). As Simoes and Gavroglu point out, Coulson might be expected to have sympathized with the *ab initio* calculations, but he didn't. Although he acknowledged that *ab initio* and semi-empirical studies may be appropriate for different kinds of theoretical activity, much of his own work was devoted to the recovery within molecular quantum mechanics of such traditional chemical notions as bent bonds and partial valence (Simoes and Gavroglu 1999, 380–389; see also Altmann and Bowen 1974, 97–105). Coulson's mathematics was designed to *suit* "chemical intuition," not annihilate or revise it.

4. The Pragmatics of Explanation. Slater and Coulson both appeal to the notion of explanation to make normative claims about the application of quantum mechanics to chemistry, but the points they make are opposed, suggesting that their views of explanation are opposed too. Slater sees the chemists' semi-empirical 'models' as *ad hoc*, and rules them out as legitimate applications of quantum mechanics because they fail to fit the paradigm of physical explanation. Coulson doesn't explicitly reject Slater-type explanation, but doubts its applicability to the new discipline of quantum chemistry. The first problem is tractability: tough explanatory ideals—like Slater's "challenge to be able to explain everything we see around us in terms of . . . fundamental theory"—are all very well, but there are trade-offs against explanatory power (measured in detailed calculation, rather than promissory notes). The second concern is consequent on this. In his 1960 critique of the 'ab initio' methods, Coulson noted that the numerical methods that were developed to address the tractability issue, and which became so powerful with the advent of digital computing, have their own drawbacks. What makes the numerical approaches yield

accurate results (e.g. large basis sets in calculating molecular wavefunctions) is precisely what makes them difficult to interpret in terms of the 'traditional' concepts of chemistry (for an account of why this should be so, see Woody 2000). This need be no defect in the view from physics, where physical explanation of chemical facts might well be revisionary: if chemical bonds don't arise naturally in accurate quantum mechanics, so much the worse for the chemical bond. Max Born, for instance, referred to chemical valence theory as 'speculation', and thought that physicists would need to calculate the binding energies of molecules to "establish the cases in which the valence theory of the chemist is reliable" (Born, quoted in Nye 1993, 229). However, Coulson identifies specifically chemical explanatory demands on quantum mechanics that are qualitative, and involve essential reference to the bond and derivative notions. The number-crunching *ab initio* studies cannot meet those demands, he argues, but quantum chemistry *should* meet them, and semi-empirical methods offer the means of doing so.

It has been known since the earliest philosophical theories of explanation that the understanding afforded by an explanation depends on features of the context in which it is given, even if the authors of those theories sought to abstract away from such pragmatic features. Given a target audience, relevant factors include the level of background knowledge assumed, the nature, presentation and plausibility of explanatory information, the salience of particular explanatory demands, and (more controversially) the explanatory relevance relation. The term 'pragmatics of explanation' is usually understood in this narrow sense, but Slater's and Coulson's perceptions of their epistemic contexts differ in a wider sense, for they were trying to do quite different things with their quantum-mechanical explanations (for an argument along similar lines as what follows, see Ramsey 2000).

For Slater, a quantum-mechanical explanation of chemical bonding is (to a first approximation) a subsumption of facts about the structure and stability of particular molecules under the quantum mechanics of systems of charged masses. (Whether his explicit view accurately reflects the discipline of physics more widely, or his own explanatory projects in solid state theory, is not a question to pursue here.) Revisionism with respect to standing theories of chemical structure and bonding is less worrying for Slater than it is for Coulson. For Slater, it is more important to get the fundamentals right from a physical point of view than it is to provide workable models of chemically interesting molecules. Slater (and Born) assume a community (of physicists) already assured that quantum mechanics is the fundamental theory governing molecular structure. This community does not need convincing of the ultimate explanatory impor-

tance of quantum mechanics with success cheaply achieved using ad hoc models.

Coulson saw himself as both a contributor to and advocate for the explanatory application of quantum mechanics within chemistry. The intradisciplinary standing of quantum chemistry could not but depend on its being seen—by chemists—to meet chemical explanatory demands. Organic chemists (to take an example) would have had fewer reasons than physical chemists to accept claims for the explanatory power of quantum mechanics with respect to chemical problems. Successful quantum-mechanical treatments of the spin states of the silver atom, say, or the spectrum of hydrogen, would not *by themselves* show that the theory had anything useful to say about molecules like benzene or naphthalene. For this reason, informative treatments of complex molecules were high on the theoretical agenda of quantum chemistry.

Stephen Brush (1999, 51–58) has analyzed how the relative standing of the valence-bond and molecular-orbital approaches evolved in the first decades of quantum chemistry. Brush argues that in the 1930s, the valence-bond approach was favoured by its presentational superiority, exemplified for instance in Pauling's visual representation of aromatic bonding in benzene, which echoed Kekulé's oscillating structure. In the 1940s, however, Coulson produced an account of bonding in benzene within the molecular orbital approach. Erich Hückel had produced the first such application to benzene in 1931, but Coulson added a matching visual representation of the molecule (the now-familiar 'double-doughnut' π -bonds). This, along with the molecular-orbital theory's superior applicability to larger molecules (and later its successful novel predictions in the case of pericyclic reactions) demonstrated, first to theoretical chemists and later to organic chemists, its superiority in accounting for the structure and bonding of organic molecules (1999, 291). Two points emerge from this, which are in tune with Coulson's agenda for quantum chemistry. Firstly, what one might call 'upward' theoretical virtues like continuity with chemical theory and explanatory power were at least as important in the eyes of chemists as 'downward' virtues like rigor in determining the relative standing of the valence-bond and molecular-orbital approaches. Secondly, supporters of the two methods accepted, by the mid-1930s, that they were equivalent in the limit of fully sophisticated treatments, but the debate continued for some time after that. Equivalence in the theoretical limit did not entail that the different ways the valence-bond and molecular-orbital theories simplified many-electron wavefunctions would yield equivalent explanations of the stability of, say, benzene. Partisans of the two approaches cited *chemical* differences between them not only because it was an argument among chemists, but also because they perceived genuine explanatory differences between the two schemes.

Were the non-revisionary semi-empirical methods developed *merely* for pragmatic reasons? Did quantum chemists like Pauling and Coulson use them only to convince skeptical chemical colleagues of the value of their subdiscipline, or the superiority of this or that scheme of approximation? There were positive epistemic reasons for a ‘retentionist strategy’ with respect to classical chemical structure. Firstly, chemical structure theory was as highly confirmed a body of theory as any in existence at the time, and theoretical continuity with that body of theory was consequently as rational as with any other. Assignments of particular molecular structures, and the general trends that govern them, had been providing explanations in spectroscopy, reaction stoichiometry and dynamics since the nineteenth century. From the chemists’ perspective, revisionism is empty posturing unless its explanatory promissory notes can be exchanged for real alternative explanations. Secondly, in two different methodological debates (valence-bond versus molecular orbitals; *ab initio* versus semi-empirical), Coulson emphasized the project of deepening and systematizing existing structural explanations in chemistry. This suggests a ‘consequentialist’ response to Slater’s charge of *ad hoc* theorizing. Although poorly motivated as instances of Slater’s program, the semi-empirical models will not be *ad hoc* if they treat trends and similarities between molecules in unified and systematic ways (based on their membership of *chemical* kinds). The unity they exhibit will, however, be local to molecular quantum chemistry.

5. Conclusion. It is sometimes argued that the successful application of quantum mechanics to the explanation of molecular structure and bonding in the 1930s and after provides evidence for the completeness of physics, and against the once popular view that the laws of chemistry are in some sense *sui generis*, or emergent (see McLaughlin 1992). A full response to that physicalist argument should address the detailed mathematical and explanatory relationships between molecular quantum chemistry and the quantum mechanics of systems of charged particles (see Hendry 1998, forthcoming). In this paper I have investigated the epistemic backgrounds which influenced the explanatory interests of physicists and chemists in the first decades of quantum chemistry. If quantum chemistry is a relatively autonomous theoretical discipline rather than an instance of a broader physical theory, the epistemic processes I have described provide a methodological explanation of why that should be so.

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