

## The Lens of Chemistry

### Abstract:

Chemistry possesses a distinctive theoretical lens—a distinctive set of theoretical concerns regarding the dynamics and transformations of a perplexing variety of organic and nonorganic substances—to which it must be faithful. Even if it is true that chemical facts bear a special (reductive) relationship to physical facts, nonetheless it will always still be true that the theoretical lenses of the two disciplines are distinct. This has consequences for how chemists pursue their research, as well as how chemistry should be taught.

Chemistry answers questions regarding the interaction of more or less stable substances, and these questions cannot be answered without the experience of these substances and of the practical conditions in which they are to be handled. —Polanyi (1958, 394)

### Introduction

Historians and sociologists of science are alive to the disciplinary interactions and overlaps between the disciplines of physics and chemistry in the 19<sup>th</sup> and early 20<sup>th</sup> centuries, and the rapid developments during that time in theories and concepts of the smallest scales of matter (Rocke 1984; Nye 1993, 1996). They discuss movements toward unification and the schools of thought that develop in their wake, just as often as they discuss numerous uprisings for independence. Disciplines are not simply arrays of axioms and experimental data, organized systematically in a fashion clearly prescribed by reason. As Michael Polyani (1958, 1966) argues, the practice of any science is transmitted from master to apprentice, as in the guilds of medieval and early modern Europe; much of what is learned is tacit in character, never

articulated, only demonstrated and imitated—and, we might add, agitated for. Disciplines are much more like countries than “fields”, their boundaries perennially in dispute. And multicultural is the rule, not the exception.

The controversy over atomism, beginning in the 18<sup>th</sup> century, is an excellent case study in this regard. Researchers concerned with it—both physicists and chemists—ranged over a wide spectrum of divergent philosophical attitudes toward the reality and constitution of atoms, as well as towards the propriety of theorizing primarily in terms of atoms. The extent of diversity has diminished to some extent today, but not eradicated. And while the dominant image of physics today in the larger academy is of a discipline that is largely philosophically monocultural—consumed with devising a single and simple “theory of everything”—chemistry is by contrast rightly regarded as thoroughgoing multicultural.

The philosophy of science is a different business from history and sociology of science. It is concerned—as is appropriate to its disciplinary logic—with the subject matter of each science rather than with its conduct or culture. It is also concerned with the relationship of their subjects—the realities to which they attend: Are chemistry and physics dealing with the same aspects of reality, or with different aspects? If the same, how should we regard their (apparently) different takes on it? Answers to these questions are meant to shed light on where we might expect each discipline to go from here, and how we might strengthen a given area of inquiry by way of educating and fostering future scientists. What instincts should be sharpened? What impulses dulled? The answers to these questions turn on whether a certain relation—the reductive relation—is true between chemistry and physics. Is chemistry in some sense redundant? Do we know yet? If not, how should chemists proceed in the meantime, for the sake of the greater good of science?

The purpose of this essay is first of all to remind the readers that, aspirational pronouncements on the part of some physicists aside, physics is a very, very long way from having engulfed chemistry—from having produced theories that render chemistry redundant. (Indeed, and this is a topic for another occasion, physics is itself a long way from being a micro-dominant monoculture. Its own relationship to “scale” is not monolithic.<sup>i</sup>) This might be because (as some voices in the philosophy of chemistry

community insist) that the subject matter of chemistry is not unequivocally reducible to that of physics—in other words that it is false that physics contains all the facts of chemistry (as it does all natural facts). I will refrain from passing judgment on this debate. Instead, I will insist that chemistry is not engulfed by physics because it is concerned with topics that revolve around theoretical subjects (importantly to do with dynamical interactions between whole molecules) typically marginalized in physics. Like physics, chemistry has its own budget of focal concerns, and these are nonoverlapping, or only marginally overlapping, with those of physics. This being the case, chemistry (like other disciplines) has to be true to its theoretical concerns, rather than to a single dogma about its relationships to other sciences, especially physics. And let the chips fall where they may. This has important consequences for chemistry education.

## Discipline Boundaries

There is a parallel between biology and chemistry that was much more prominent in the 19<sup>th</sup> century than it is today. Biology's task is to bring intellectual order to the bewildering variety that is life on planet Earth. It succeeds in this task by systematic application of the axiom that the diversity of life on the planet is organized by a unifying principle of natural history (thanks to natural selection, taken together with a small handful of population-statistical principles), having sprung as it must have from a small handful of seeds—possibly even just one seed. The tree of life is the guiding image of order in biology.

Just as biology undertakes the taxonomy, with explanations, of the diversity that is life on this planet, chemistry has taken upon itself bringing intellectual order to the varieties of (nonliving) substance, on the presumption that there must be an axiom or unifying principle that makes this too possible. But what is that unifying principle? When Dmitri Mendeleev first presented his table of the elements to the Russian Chemical Society in 1869, he defended it on the basis of eight fundamental premises, premier among them was the principle that the properties of elements are in periodic dependence upon their atomic weight—an important corollary of which is that certain groupings of the elements were based

upon their chemical combining or “bonding” powers. Still, there is nothing so simplifying or unifying in chemistry as the theory of evolution by natural selection in biology.

One notable idea, underlying many pronouncements of many physicists regarding the status of chemistry, is that the order in chemistry must spring from the fact that there are a small handful of fundamental building blocks of matter (more fundamental even than the elements themselves), and that their combinations and interactions are governed by an even smaller handful of principle or laws. This is why it has been tempting to think of chemistry as a footnote to physics: insofar as chemistry is interesting, that interest derives entirely from its unavoidably close relation to physics. Chemistry must be a derivative enterprise. And hence P.A.M. Dirac can proclaim:

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved (Dirac 1929).

But there are important disanalogies too between chemistry and physics—which are at the root of certain tensions I will be discussing in this paper. Here are some key examples. (1) The basic unit of dynamic in chemistry is the reaction, whereas in physics it is the force and the corresponding change wrought by it in a given body’s momentum: chemistry is characteristically concerned with larger processes than physics is—involving a greater number and variety of substances. (2) Chemistry is also concerned with the differences between the substances that enter into reactions, as wholes, rather than with components taken individually—even though it recognizes identical components. In other words, chemistry is concerned with how different substances interact, as wholes, rather than with how like substances might interact on the most minute scales—whereas physics is at best equally concerned with both. One final example: (3) Chemical reactions have characteristic time horizons, so chemistry takes an interest in the time scales of processes, and focuses upon a characteristic scale, whereas this issue holds no inherent interest in physics. All these things suggest fundamental differences of orientation between

chemistry and physics. And that it would be a mistake simply to view the one as operating closely within the orbit of the other. Or to view them as operating with the same lens. The key to understanding the place of chemistry in the scientific pantheon is to understand the lens of chemistry—to locate its intellectual concerns in relation to those of its scientific neighbors. The present paper seeks to do exactly this, and to locate at least some of the challenges of chemistry education as proceeding from chemistry's self-situation in relation to its scientific neighbors.

## The Image of Chemistry in the Philosophical Lens

J. S. Mill was attuned to the differences of principle between chemistry and physics in his highly systematic approach to the philosophical foundations of science:

I shall give the name of the Composition of Causes to the principle which is exemplified in all cases in which the joint effect of several causes is identical with the sum of their separate effects.

This principle, however, by no means prevails in all departments of the field of nature. The chemical combination of two substances produces, as is well known, a third substance with properties entirely different from those of either of the two substances separately, or of both of them taken together. Not a trace of the properties of hydrogen or of oxygen is observable in those of their compound, water. The taste of sugar of lead is not the sum of the tastes of its component elements, acetic acid and lead or its oxide; nor is the color of green vitriol a mixture of the colors of sulphuric acid and copper. This explains why mechanics is a deductive or demonstrative science, and chemistry not. In the one, we can compute the effects of all combinations of causes, whether real or hypothetical, from the laws which we know to govern those causes when acting separately; because they continue to observe the same laws when in combination, which they observed when separate: whatever would have happened in consequence of each cause taken by itself, happens when they are together, and we have only to cast up the results. Not so in the phenomena which are the peculiar subject of the science of chemistry. There, most of the uniformities to which the causes conformed when separate, cease altogether when they are conjoined; and we are not, at least in the

present state of our knowledge, able to foresee what result will follow from any new combination, until we have tried it by specific experiment (Mill 1874).

This did not lead Mill to disparage a rightful place for chemistry among the sciences, as an independent discipline. Indeed he wrote specifically, in the paragraph immediately following the passage just quoted, that “there is no reason to despair of ultimately raising chemistry...to the condition of deductive sciences”. All it takes is articulation of the appropriate “laws” as he called them—and thought they were structurally of a different basic form—by which the phenomena they describe operate.

Mill’s optimistic attitude towards the discipline of chemistry has never been popular among physicists.<sup>ii</sup> Herbert Dingle, for instance, infamously proclaimed:

[T]he truth is that chemistry indeed has not place in the strict scientific scheme, and that this is so can be seen from the fact already evident even at the present stage of scientific progress, that the ultimate generalizations of chemistry are all derivable, and indeed must inevitably have been reached sooner or later, from the development of physics itself—chiefly the departments of optics and electromagnetism. The periodic table, originally a product of chemical research, is a product also of spectroscopic research, and with this difference, that instead of showing in each place a chemical symbol and an atomic weight, the spectroscopic table shows a configuration of electric charges which, when fully, understood, will undoubtedly prescribe all the varieties of chemical combination that are possible. The whole of chemistry may therefore, so far as final results go, be regarded as a superfluous study (Dingle 1952, 210).

This position echoes the oft-quoted remark of Dirac quoted earlier in this essay. And it resonates with the model of unity in science that originated within the Vienna Circle, with roots in conceptual analysis.<sup>iii</sup> The model, first developed by August Comte, culminated in Rudolf Carnap’s *Logical Foundations of Probability* (1928). On this conception, the sciences are unified through the unity of their subject matters (which ultimately constitute one real world), which is evident in the relations between their concepts. Roughly, scientific terminology makes reference to the world, perhaps even to the same regions of it, but different

sciences make contact with the world at different “scales,” “levels,” or “strata”. And this fact corresponds to the relations in which stand the conceptual apparatus of different sciences: the concepts of the sciences stand in hierarchy relations, corresponding to the hierarchy of the sciences themselves, and this hierarchy is organized roughly along the lines of scale and complexity—paradoxically concepts involving higher scales and complexity given over to disciplines lower on the scientific hierarchy.

Carnap’s own work was characterized by a concern for logical constructions out of basic concepts defined by an axiomatic framework, and rigorous reductive logical connections between certain conceptual categories. This orientation led him to a privileging of a “most basic stuff” and a preference for physics as a privileged locus of “first principles”. And this consequently led him to a hierarchy of conceptual structures for the sciences.

But this reductive program ultimately proved generally infeasible as a way of conceptualizing the sciences. And eventually different philosophical programs vis-à-vis the sciences grew up in its place, around such labels as “emergentism” and “supervenience.” The enormous literature on failed proposed reductions is an eloquent corroboration of Mill’s catholic position by contrast with Dingle’s arrogantly exclusivist one. Because the “math” between the whole and its parts is not a simple sum, however construed. In the minds of many, however, and perhaps due to pronouncements such as those of Dirac and Dingle, it has seemed that the reductionist program vis-à-vis just chemistry has been more successful. It has seemed as though the areas of overlap between chemistry and physics is unusually broad, their topics unusually close. There is, after all, those areas now referred to as chemical physics and physical chemistry, which appear to unite the two fields in an unstinting way. After all, they have combined forces to produce a unified theory of atomic structure.

But this harmony between chemistry and physics, in the figure of atomic theory, must not be oversold. First of all, it is not at all obvious that the conceptions and principles articulated in contemporary theory of atomic structure can all be said to belong to the discipline of physics in a proprietary way. For instance, it isn’t at all clear that any theory of chemical bonding (whether resonance theory or its rival molecular orbit theory) can belong entirely in the domain of physics—for reasons that

will come out somewhat later in this essay. Moreover it is clear that the bulk of what chemistry deals with—namely, chemical reactions—can never be reduced to principles of physics (for discussion of this point see van Brakel 2000, chapter 5). And finally—and really quite importantly—chemists and physics in the 19<sup>th</sup> century did not share the same conception (indeed there was considerable discussion of the “chemical atom” as contrasted with the “physical atom;” Rocke 1984 and Nye 1993 discuss these differences *passim*.) And so the status of chemistry as special handmaiden to physics is very much in doubt—just as much as that status is in doubt for any other scientific discipline.

A key element in the case against reduction of chemistry to physics lies in the structure of matter and the relation of such structure to bulk properties of the substance. Properties and behaviors of matter at medium scales—indeed at the scale of molecules—depends on a great deal more than merely those physical qualities pertaining to their parts and the principles that govern their combination. How they combine is also enormously important for taxonomic purposes—this is the lesson (at least in part) we can learn from isomers. (And Mill is right: who could have predicted this in advance of seeing it whether—and how, and in how many ways— $N$  substances will combine to form  $M$  products?) Even so, when once we know whether (and how) combinations may occur, we still have don't have access to its bulk properties or the kinds of processes they enter into.

So consider isomers: isomers are molecules with the same numbers of the same atomic elements (and hence the same chemical/atomic formula) but which differ in behaviors or characteristics. There are several categories of isomers—some are merely structural (where the chemical bonds are between different components), others involve the same bonds, but they are differently organized in space (they are stereoisomers, that can be divided further into geometrical and optical subcategories). In addition to theorizing about how parts of such molecules manage to combine to form the whole, it is also chemistry's job to explain the variety and differences in their behavior—so many enter in a vital way into the chemistry of respiration and other physiological processes of living things. And while it is quite true that quantum principles help with answering questions as to whether different components combine and what into, it is nowise true that they have been equally helpful with answering questions as to the differences



between isomers.

In fact, the latter questions—how differences in structure parlay into differences in behavior—are intertwined with issues that have caused physics itself serious theoretical headaches from the very first, and which persist to this day. Questions as to the bulk properties of matter, and their relations to thermodynamic behavior, are still unsettled. And chemistry has a part to play in that story as well.

## Rival Strategies in Chemistry

Early eighteenth century chemistry postulated a substance called phlogiston, whose release accounts for a substance's combustibility in the first instance, and accounts also for the difference (the loss) in weight between the combustible and its residue. This principle of flammability was also thought to give metals their luster and ductility. According to the theory, all flammable materials contain phlogiston that is liberated in burning, leaving the "dephlogisticated" substance in its "true" calx form.

Enter Antoine-Laurent Lavoisier. His scientific genius was to perform exacting systematic determinations of the weights of reagents and products involved in chemical reactions, including the gaseous components. He demonstrated that in all cases of combustion where a product weighed more than the original reagents, air was absorbed, and that when a calx was burned with charcoal, air was liberated. For instance, he determined precisely the weight of a mercury (II) oxide, a red powder, in a sealed container. When the container was heated, so that the powder changed to a silvery liquid—metal mercury—, the weight of the products (liquid mercury plus air) equaled the weight of the original oxide. And he was able to produce the reverse reaction: air combined with the mercury metal when heated produced mercury oxide. This confirmed for Lavoisier the axiom that matter is conserved through any reaction—an axiom he had formulated after noticing that the weight of a candle together with the air in a jar equaled the weight of the all the products after burning. Conservation of matter was contrary, by his reckoning, to the theory of phlogiston—since one would have to assign a negative value of matter to

phlogiston. And Lavoisier's conception of the constitution of air provides the modern basis for an understanding of combustion and respiration as caused by chemical reactions with the part of the air that Lavoisier himself called "oxygen."

The exacting experimental methods Lavoisier devised and taught, and his definitive proof by composition and decomposition that water is made up of oxygen and hydrogen, crystallized the modern science of chemistry. His assignment of new names to substances—most of which are still used today—played an important role in advancing the so-called Chemical Revolution, in part because the names were a vehicle for conveying the quantitative theory behind them. Chemists today teach that combustible materials (including unruined metals) are "deoxygenated" when in their pure form and become oxygenated when burned. And that the weight of oxygen makes up the difference.

Lavoisier's systematic treatment of chemical processes, involving the application of heat, led naturally to rejection of phlogiston, and thereby to joint (unified) treatment of combustion and many other chemical processes, including respiration, under a single embracing (unifying) theory. Lavoisier's strategy of analysis is a reductive strategy—very much in the spirit of the Newtonian program. Indeed Newton had himself set down the outlines of this reductive, physicalist program, in the preface to the first edition of the *Principia*:

I wish we could derive the rest of the phenomena of Nature by the same kind of reasoning from mechanical principles, for I am induced by many reasons to suspect that they may all depend upon certain forces by which the particles of bodies, by some causes hitherto unknown, are either mutually impelled toward one another and cohere in regular figures, or are repelled and recede from one another. These forces being unknown, philosophers have hitherto attempted the search of Nature in vain; but I hope the principles here laid down will afford some light either to this or some truer method of philosophy (Newton 1952).

Lavoisier's program was wildly successful at unifying and energizing chemistry—perhaps as successful as Newton's principles were for mechanics.

But the history of chemistry, especially in its early days, is really one of rival analytical strategies. The reductive strategy (for instance as Lavoisier employed it) was to build up a catalog of elemental building blocks, then to identify substances as the sum of their elemental building blocks. The point I wish to make at this juncture, however, is that this strategy has its limitations. And chemists were among the first to notice. Illuminating the interplay between the reductive strategy and its limitations, within the discipline of chemistry, can help us identify the characteristic lens of chemistry—what is distinctive about chemistry, and how this lens situates chemistry within the space of its scientific neighbors. I use the term “lens” because it admits of a natural distinction between that which is “in focus” and that which is allowed to remain unfocused. The “lens” of a discipline embraces the totality of its concerns, but some of its concerns enjoy a place of honor, in “focus”, so that their image is more sharply defined there than are concerns outside the focal space.

Many chemists were very early on very critical of reductionist strategy as the sole analytical strategy of chemistry—some to the point of rejecting the very idea of atomism (Duhem and Ostwald, for instance, see Rocke [1984, 325ff]; for philosophical elucidation of Duhem’s philosophical and ontological orientations see Wilson [mss, preprint]). These strategies were, at least early on, very unsuccessful in handling questions regarding which elements will combine, and the properties of the resultants. The important point to notice is that many chemists were also prepared to adopt a host of alternative analytical strategies in dealing with these questions. Ostwald and Duhem, for instance, agitated for thermodynamic (nonmechanical, and nonstatistical) foundations for the theory of substance, with the concepts of heat and entropy entering as independent variables. Nor were these the only options (Nye 1993 and Rocke 1984 describe a much larger array). The condition of the enterprise of physical chemistry at the end of the 19<sup>th</sup> century was one of plural research strategies, as well as disunity.

Still, this is not to say that there was nothing to unite the multiple scientific enterprises going under the “chemistry” label: they share, among other things, a common core set of questions and disciplinary values. As Nye (1984, 3) writes, a “programmatically conceptual core of chemical thought from the eighteenth century through the twentieth century was what I call the problem of the dynamics of

matter (What holds a substance together? What makes it change?).” What Nye does not say—and what I wish to emphasize here—is that this problem has a very strong analog in physics—in the pure theory of thermodynamics, without regard for the identities of substances. This is the problem of how to understand the major concepts of thermodynamics (such as heat, temperature, entropy and equilibrium)—and whether this was possible in purely mechanical terms. This problem does not, however, seem to provide a conceptual core to the discipline of physics—it does not lend physics a special lens. Chemistry, by contrast, views the problem rather differently. Let’s take another look at the history.

The caloric theory of heat, for instance, held that heat consisted of a fluid called caloric, that could be transferred from one body to another, but neither created nor destroyed in any physical process. Caloric was the “subtle fluid” introduced by Lavoisier himself, upon the ouster of phlogiston, to help make his sums work out; and he was among the first to measure heat exchange using a calorimeter. Ultimately Joule and others would show that mechanical work against a force of friction produces heat—that there is a mechanical equivalent of heat. Of course this refutes the fluid model of heat—at least refuting heat’s status as something that is neither created nor destroyed, and so as a kind of matter. Conventional wisdom now has it that the mechanical theory of heat enters upon the historical stage around 1850, unifying the treatment of heat with the range of known mechanical phenomena (especially with Joule’s and Mayer’s independent discoveries of the mechanical equivalents of heat), and in the process ousting the notion of caloric.

The trouble with this conventional wisdom is that resistance to the mechanical theory of heat—and there is rather more resistance than conventionally recognized, mostly neglect (as I’ll discuss presently)—is made invisible, and with it the chemist’s lens. That resistance is not resistance to the unification wrought by a mechanical theory of heat—similar to the unification wrought by the ouster of phlogiston. The move to expunge caloric is a reductive move essentially—and so essentially not something that springs from a concern for a theory of the dynamics of matter (to reiterate Nye’s phrase). The ouster of caloric thus does not stem from the chemist’s lens. And that this fact explains the type of resistance it encounters. (Of course there is nothing wrong with such a move in principle. As a strategy,

it is without peers.) The point is simply that the move to oust caloric could not succeed without backing of a certain sort—in spite of its reductive credentials.

When Daniel Bernoulli (1738) published his book *Hydrodynamics* considerably earlier in 1738, he proved that gas pressure—which he defined (as a good dynamicist) in terms of collisions with container walls—is two thirds the average kinetic energy of the gas in a unit volume. There he gestured at a principle of conservation of energy—something within the orbit of a physicist’s lens. This theory had all the hallmarks of a good reductive mechanical theory, but it had nothing over the notion of caloric. Chemists paid it little heed. Caloric theory persisted—and flourished—because of its impressive conceptual value within the chemist’s framework. And beyond, into the theory of thermodynamics—as now we will discuss.

Sadi Carnot, in the 1820’s, wrought the first theory of the steam engine. His idea was that just as water flows downhill, caloric flows from hot to cold: and the steam engine utilizes this caloric flow just as a water wheel takes energy from falling water. His analysis led to many correct conclusions, such as that the amount of work that a given amount of heat would provide depends only on the size of the temperature drop, and that there is a limit to how much work could be extracted. Carnot proved that the limit was the work provided by a reversible engine, one with no friction and heat exchange only between objects at the same temperature. Unfortunately, Carnot died very young, and his work was almost unknown until the 1850’s, when the mechanical theory of heat was gaining converts, and the caloric theory was (at least according to historians of science) disappearing. But was it?

In his 1910 presidential address to the Physical Society of London, H. L. Callendar expressed reservations to the expunging of caloric, and maintained that the theory of caloric as developed by Carnot:

leads immediately to the correct solution of the relations between heat and motive power (energy or work) in all reversible processes, and appears to be in some respects preferable to the mechanical theory as a method of expression, because it emphasizes more clearly the distinction first clearly stated by Carnot, between reversible and irreversible transformations, and because it directly provides the natural measure of

a quantity of heat as distinct from a quantity of thermal energy (Callendar 1910).

Whereas Joseph Priestley's reservations to abandonment of caloric are invariably expressed in terms of his own preferences for the theory of phlogiston's accommodations (of the same phenomena as his opponents cite against him<sup>iv</sup>), Callendar's resistance to abandoning caloric is quite different. It's substantially a philosophical one, very much in the spirit of antiatomist chemists: his preference for Carnot's formulation of the caloric principle proceeds from the fact that the theory of caloric illuminates an important—not to be neglected if you're a chemist—demarcation between reversible and irreversible processes. This is a preference for how to handle the difference between reversible and irreversible—a preference to maintaining a strong taxonomic barrier between the two. Callendar's presidential addresses thus expresses a certain taxonomic concern—a concern for valuation of certain boundaries that divide processes at a scale that matters to chemists. He was favoring the preservation of a bright line between two important thermodynamic categories, over the that can be wrought through ouster of caloric. Though a physicist by training, Callendar's instincts lay with retaining the valuable chemist's lens that the theory of caloric exemplified. I will say more about this lens in the next section.

The theory of caloric could fade from the scene only when a comprehensive thermodynamic theory became genuinely useful—useful for the purposes of chemistry too. A theory that preserved the distinctions important for a theory of the dynamics of matter. Only then could caloric be ousted and mechanical heat prevail. (By the way, it is not entirely clear that this has in fact taken place. These questions are still very unsettled in physics itself.)

As these cases discussed above suggest, there is some conflict of instincts between physics and chemistry. Tidiness and sparseness—the instinct favored by a number of (though by no means all) physicists—can be at odds with scrupulous attention to taxonomy—the chemist's perennial compulsion. This holds true even as regards the question of atomism. While it was the chemist's instinct to “invent” atoms because they facilitate the taxonomy of substance—because they make for good housekeeping—the invention does not stop the chemist from inventing also a taxonomy of isomers—at one stroke

vindicating the chemist's project and ruining the reductionistic moment that atomism occasions.

And so, while it is quite correct to maintain that quantum theory throws important light on atomic structure, that light owes a great deal to the concerns of chemists for faithful taxonomy. Coulson described the first decade of scholarship in quantum chemistry, working towards the theory of chemical bonding, as work spent "escaping from the thought-forms of the physicist, so that the chemical notions of directional bonding and localization could be developed" (see Nye 1993, 279). In other words, at least some aspects of modern theories of chemical bonding owe much less to the physicist's characteristic concerns of physics than to those of chemistry. And even that light is not strong enough to illuminate chemical reactions and transformations very generally. Hans Primas emphasizes that molecular structure, as such, is a classical not quantum idea, and as such foreign to the founding principles of quantum mechanics which "neither gives a correct nor a consistent description of molecules. Quantum mechanics gives perfect predictions for all spectroscopic experiments. However, chemistry is not spectroscopy" (Primas 1980, 105). So what exactly is chemistry?

## The Lens of Chemistry

A successful physics of the universe should of course provide a catalog of the building blocks of matter (assuming there are such building blocks<sup>v</sup>) and then proceed to lay down the governing principles by which they interact. And if that's all there is to the universe, then physics is the only science we need. And reductive intellectual instincts are all a scientist should ever require. That a chemist's instincts are at some odds with this tidy proposal is importantly suggestive. There is a tension. Although not opposed to reduction in principle, chemistry, it seems, will embrace fully exactly those reductions that throw light on and preserve a faithful rendering of those topics at the center of its concerns (the structure and dynamics of matter, and its transformations), while holding other proposed reductions at arms' length. Perhaps the most diagnostic case for examining this tension is ultimately that of the relationship between chemistry and quantum theory.

There is substantial controversy as to whether the structure of matter, as described by chemistry, is reducible to quantum theory. On one side there are those who, like McLaughlin (1992), argue that quantum theory provides a comprehensive basis for a theory of chemical bonding and chemical structure, so that we have reason to maintain that chemistry is in fact ontologically reducible to quantum mechanics—the facts discussed by chemistry are fundamentally quantum-mechanical facts. By contrast there is Primas's position that we encountered above, articulated in Scerri as follows:

the periodic table, the central classical explanatory model of the chemist, has not been deduced from quantum mechanics. All that can be done is to give a quantum mechanical justification for electronic configurations that are obtained empirically from atomic spectra. One cannot begin with quantum mechanics alone and predict the configuration of a particular atom (Scerri 2007, 74-75).

Hendry maintains yet another distinct position:

Rather than an explanation of chemical structure by physical theory there was a joint venture: the explanation of various facts by the use of quantum mechanics applied to a given molecular structure. There was no mesh or interface between the quantum mechanics and chemistry, at least none that required explanation. What we had was an instance of quantum chemistry, the quantum theory of atoms and molecules (Hendry 2006, 187).<sup>vi</sup>

What I wish to emphasize here is that it is really immaterial whether ontological reductions of the sort McLaughlin (1992) defends has been achieved in the “merger” of chemistry with quantum physics (as Hendry 2006 would call it, or hybridization between chemistry and quantum theory as Vemulapalli 2006 would call it). Because the focus of chemistry will be what it is whether or not the reduction holds—and this focus is distinct from that of physics. The evidence for this is abundant. As Scerri writes:



[t]he highly accurate quantum chemistry calculations are empirically very adequate and yet chemists continue to rely on classical explanatory models such as Lewis structures and VSEPR theory to name just two examples. The fact that they do so is also not surprising since these models and concepts operate at the appropriate chemical level which is familiar to chemists, namely the talk of pairs of electrons, atoms, and bonds. By turning to quantum mechanics the chemist can generate quantitative values for bond angles, bond strengths, or dipole moments, but such calculations are not a substitute for the classical explanatory schemes which continue to be used by chemists (Scerri 2007, 74).

The point I wish to make is simple: chemistry focuses on certain aspects of matter—it is concerned with matter at a particular scale, namely the scale at which reactions and transformations show up as meaningful events. Any theory that would blur the sharpness of these events is received by chemistry with caveats and cautions; for it cannot be embraced unconditionally within the chemical context. Since it might “blur” the focus. For chemistry is concerned with a certain range of phenomena (again: those pertaining to the dynamics and transformations of matter). This requires chemistry to treat events occurring at lower scales integratively, so as to capture the correct aspect.

The reductive impulse—the intellectual orientation stereotypical of the physicist—seeks to break things down into totally independent parts, as well as totally independent principles of interaction. Whereas the integrative impulse—characteristic of the chemist vis-à-vis lower scale events—is to taxonomize and correlate behaviors with whole units of substance in context. This impulse seeks to situate behaviors in their context. In chemistry, this impulse manifests in the “resistance of some contemporary chemists to the reduction of the chemical molecule to an isolated physical molecule” (Nye 1993, 280). R G Woolley and Hans Primas exemplify this impulse. Woolley, for example, stresses that quantum mechanical calculations of molecular characteristics must presuppose a nucleus “in isolation” (in the Born-Oppenheimer approximation): here nuclei are treated (unrealistically) as inhabiting equilibrium positions. Molecular properties, on Woolley’s view, are not possessed intrinsically by the molecules that

manifest them; molecular properties—such as the shape of a molecular—are properties of situated rather than isolated entities. They are properties of dynamical rather than stationary entities, and so we require the development of new theoretical tools to predict molecular shape.

The quantum mechanical analysis of the idea of molecular structure that I sketch here is partly an attempt to make clear the fact that quantum theories of the physical and chemical properties of bulk matter could not have been developed to their present-day form without borrowing the notion of molecular structure from classical chemistry. One cannot therefore claim that the hitherto mysterious structural concept underlying chemical explanation is derivable from physical theory and therefore “explained” by quantum mechanics (Woolley 1978, 1074).

The chemists’ instincts vis-à-vis events at a lower scale than that characteristic of their lens is thus better aligned with has elsewhere been called Systemism (Thalos 2011). A System, on this view, is not simply a network of independent entities standing in some random set of (“external”) relations to one another—at a level superordinate to that in which its components are rooted. A System is, rather, a network of entities that stand in “nonelective” bonds to one another. These are the internal relations. What I mean by the term is this: it is not possible to assemble the entities in question, as a System, without also the bonds figuring in; it is not possible to assemble the entities in question, as a System, with arbitrarily-chosen bonds. The bonds in question are ineliminable to the confederation of these entities, even if some of these entities can confederate, with other entities, to form a still different sort of System. The relations between the entities in question are thus “internal” to their confederation. The bonds are therefore also an ineliminable aspect of an apt analysis of their Systemhood.

This idea—that structuring relations are what make a System what it is, and so swapping out elements that can be swapped out without changing this structure would leave the System unchanged—this idea is basic to the theory of Complex Systems, and in some ways core as well to study of networks (which will be discussed again in the next section). It is why Systems Theory is a study of dynamics—of

behavior—rather than of primarily static features. For on the Systems view, behavior is not “external”—not simply an accident of circumstances, or even of independent laws governing interactions “externally”; rather, behavior is characteristic; behavior is defining. This is an insight worthy of a chemist. Indeed in the conclusion to her book on the development of chemistry as a discipline in its first 150 years (1800-1950), Nye (1993, 281) writes: “The emphasis on environment and on the molecule acting in an environment is not trivial, for it lies at the heart of the conceptual aims and problems of the chemical discipline, as outlined in this book.”

Thus the chemist’s focus on the properties and interactions of bulk matter in macro (and ultimately also biological contexts) puts her at odds, in some respects, with her physicist counterparts. She is obliged to be faithful to this “scale” of behaviors, even if she must blur or distort the image of other scales in her lens. This, as we’ll discuss shortly, does not keep her from borrowing; in fact, it impels her to do so.

## **We are all Chemists now**

Today we are more mindful than ever of the profound effects of interlinking. Individuals can behave quite differently when linked to others (whether identical or different from themselves), especially when networked with many others. Of course we humans have always been socially networked, but the Internet and its globalizing effects has made us much more aware of the impact of connections, in the process of enlarging and heightening their impact. Networking enhanced by information technology has amplified some effects while damping others: our neighborhoods have grown bigger (because we can connect to almost anyone on the face of the globe at near-light speed) but at the same time our world has grown to seem smaller (because the overlaps in our neighborhoods are so large). Network conditions can magnify and telescope effects, or alternatively they can diminish or even totally extinguish them. But even more crucially: which they will do is exceptionally hard—if not positively impossible—to predict.

Everything depends on the characteristics and architecture of a network—how connected, how clustered, how diffuse, how ghettoized. And all of these facts are as true of elementary and subatomic particles as they are true of social entities—if not more so. The impacts of network architecture and characteristics are currently being investigated by sociologists, ecologists, biologists, mathematicians, physicists, computer scientists and economists. Networks are now in the foreground in nearly all regions of intellectual investigation—from societies of living things, to planets orbiting their star, to electrons in a Bose-Einstein condensate—and their mathematics has become a large and diverse industry.<sup>vii</sup>

But chemistry has been attuned to this insight for a long time now. Chemists are admirably humble, not presuming a facile answer to the question as to what can be expected from a substance with one more or one less electron, or with more or less energy. Chemistry has always occupied a critical place in the scientific disciplines—it has occupied a place where the regime of individual (and presumed independent) entities intersects that of the collective and networked. The theory of networks is now exploring this territory in its own distinctive ways. But chemistry has never been able to avoid the fundamental intersection between the individual/independent and the collective/networked. Chemistry has been, for the greater part, about the affinity between things—about the spark that brings together like and unlike, and the give-and-take between things. Indeed chemistry is about nothing at all if not the nonlinearities that happen when many things aggregate. Bringing these facets to the foreground is the function of chemistry's lens. And chemistry education might well benefit from bringing these topics explicitly together. Teaching the principles of network theory to chemistry students might well facilitate their navigation of the boundaries of their discipline; it might make them more sensitive to tensions at discipline boundaries, and more aware of the large variances of “focal length” they in particular are bound to encounter in their researches and in their intellectual journeys.

## Teaching Good Chemistry

Robert Mulliken remarked that “chemists love molecules, and get to know them individually,” while by contrast, “physicists are more concerned with the fields of force and waves than with the individual personalities of molecule or matter” (as quoted by Schweber 1990, 403-4; Nye 1993, 281). Indeed, among the most important diagnostic instruments in a chemist’s laboratory are the chemical substances themselves—both the objects of study and the means of study. Organic chemists in particular, especially early on, prided themselves on a “chemical feeling” (Nye 1993, 268) that came with their work in the laboratory. Of course these observations point to the importance of laboratory work for chemistry and chemistry education. But they also point to an instinct that requires fostering in the discipline’s initiates. It is an instinct for appreciating the conceptual “boundaries” between one substance and another—an instinct that few physicists anywhere exemplify. This instinct is shared with many biologists—especially those that make it their business to focus on just a few organisms. This strategy of inquiry puts special emphasis on drawing out the larger lessons of particularities.

Teaching this strategy of inquiry and analysis is especially difficult. Since particularities are—true to name—so particular. So it presents a special challenge to chemical education—to teach the fundamentals of a discipline whose lens focuses on particularities in this way. The discipline of chemistry seems to have confronted this challenge in a number of different ways. One key strategy for meeting this challenge has been what we might call its “multicultural” stratagem. Nye describes the inclusive nature of theoretical chemistry as an “interdisciplinary science”:

Our history has shown us how some leaders of research groups aspire to do more than direct their workers in the straightforward applications of disciplinary practice that we have learned to call “normal science.” Rather, choosing to address the unsolved problems that are part of the disciplinary core, the group reaches out to incorporate ideas, techniques, and materials from specialties and disciplines other than their own (Nye 1993, 272).

A culture of inclusiveness—of fostering exploration of principles and techniques found elsewhere—is the legacy of chemistry. The rest of science would do well to emulate it.

Perhaps more valuable still, for chemistry students, would be a recognition that their lens really does differ from the lens of physicists—and biologists too, obviously. Appreciating that a chemist's core concerns bring distinctive features of nature into theoretical focus is an invaluable philosophical asset. It can make the difference between confidence in one's tools and lack of confidence in the principles of chemistry research itself. And this is ultimately the difference that philosophy can make.

## References

- Batterman, R.: 2008, Intertheory Relations in Physics, The Stanford Encyclopedia of Philosophy, E. N. Zalta (ed.), <http://plato.stanford.edu/archives/fall2008/entries/physics-interrelate/>
- Bealer, G.: mss, Analysis and Definition.
- Bernoulli, D.: 1738, Danielis Bernoulli Joh. Fil. Hydrodynamica, sive, De viribus et motibus fluidorum commentarii, Argentorati: Sumptibus Johannis Reinholdi Dulseckeri, typis Joh. Henr. Deckeri, Typographi Basiliensis.
- Callendar, H.L.: 1910, The Caloric Theory of Heat and Carnot's Principle, Proceedings of the Physical Society of London, 23, 153-189, Retrieved from <http://www.iop.org/EJ/abstract/1478-7814/23/1/315>
- Carnap, R.: 1928, The Logical Construction of the World, R. George (tr.), University of California Press, Berkeley.
- Cat, J.: 2007, The Unity of Science, The Stanford Encyclopedia of Philosophy, E. N. Zalta (ed.), Spring 2009 ed.
- De Morgan, A. & De Morgan, S. E.: 1872, A Budget of Paradoxes (Reprinted / ed.), London, Longmans, Green.
- Dingle, H.: 1952, The Nature of Scientific Philosophy, The Scientific Adventure (pp. 210), Pitman and Sons, London, 210.
- Dirac, P.A.M.: 1929, Quantum Mechanics of Many-Electron systems, Proceedings of the Royal Society of London, A123, 714-33.
- Hendry, R.F.: 2006, Is There Downward Causation in Chemistry? In The Philosophy of Chemistry: Synthesis of a New Discipline, D. Baird, E. Scerri & L. McIntyre (eds.), Springer, The

Netherlands, 173-89.

Jackson, M.O.: 2008, *Social and Economic Networks*, Princeton University Press, Princeton, NJ.

McLaughlin, B.: 1992, *The Rise and Fall of British Emergentism*. In A. Beckerman, H. Flohr & J. Kim (eds.), *Emergence or Reduction? Essays on the Prospect of a Non-Reductive Physicalism*, de Gruyter, Berlin, 49-93.

Mill, J.S.: 1874, *A System of Logic, Ratiocinative and Inductive : Being a Connected View of the Principles of Evidence and the Methods of Scientific Investigation* (8th ed.), Harper & Brothers, New York.

Newman, M.E.J.: 2010, *Networks: an Introduction*, Oxford University Press, Oxford, New York.

Newman, M.E.J., Barabási, A.-L., & Watts, D. J.: 2006, *The Structure and Dynamics of Networks*, Princeton University Press, Princeton, NJ.

Newton, I.: 1952, *Philosophiae Naturalis Principia Mathematica* (1687), A. Motte (tr.) M.J. Adler (ed.), William Benton, Chicago.

Nye, M.J.: 1996, *Before Big Science: The Pursuit of Modern Chemistry and Physics, 1800-1940*, Twayne Publishers, New York.

Nye, M.J.: 1993, *From Chemical Philosophy to Theoretical Chemistry*, University of California Press, Los Angeles.

Nye, M.J.: 1984, *Introduction. The Question of the Atom: From Karlsruhe Contress to the First Solvay Conference, 1860-1911*, Tomash Publishers, Los Angeles.

Polanyi, M.: 1958, *Personal Knowledge: Towards a Post-Critical Philosophy*, University of Chicago Press, Chicago.

Polanyi, M.: 1966, *The Tacit Dimension*, Doubleday, New York.

Primas, H.: 1984, *Foundations of Theoretical Chemistry*, in R. G. Wooley (ed.), *Quantum Dynamics of Molecules*, Plenum Press, New York, 39-113.

Priestly, J.: 1796, *Considerations On The Doctrine of Phlogiston and the Decomposition of Water*, Retrieved from <http://web.lemoyne.edu/~GIUNTA/phlogiston.html>

Rocke, A.J.: 1984, *Chemical Atomism in the Nineteenth Century*, Ohio State University Press, Columbus.

Schweber, S.S.: 1990, *The Young Clarke Slater and the Development of Quantum Chemistry*, *Historical Studies in the Physical and Biological Sciences* 20, 339-406.

Scerri, E.R.: 2007, *The Ambiguity of Reduction*, *HYLE – International Journal for Philosophy of Chemistry*, 13 (2), 67-81.

Strogatz, S.H.: 2003, *Sync: The Emerging Science of Spontaneous Order* (1st ed.), Theia, New York.

Thalos, M.: forthcoming, *Without Hierarchy*, Oxford University Press, New York.

Thalos, M.: 2011, *Two Conception of Fundamentality*, *Philosophy of the Social Sciences*, 41:2, 151-177.

Van Brakel, J.: 2000, *Philosophy of Chemistry*, Leuven University Press.

Vemulapalli, G.K.: 2006, *Physics in the Crucible of Chemistry*, In *The Philosophy of Chemistry: Synthesis of a New Discipline*, D. Baird, E. Scerri & L. McIntyre (eds.), Springer, The Netherlands, 191-204.

Wilson, M.: mss preprint 2007, *Duhem Before Breakfast*, PhilSci Archives.

Woolley, R.G.: 1978, *Must a Molecule have a Shape?*, *Journal of the American Chemical Society*, 100,

1073-78.

- 
- i Thalos (forthcoming) advances this thesis.
- ii J. van Brakel (2000,15) attributes to Mill—mistakenly, to my mind—the view that chemistry is a failed science. I have quoted Mill at length to allow him to speak better for himself.
- iii Bealer [mss], gives a penetrating treatment of the relationship between these ideas, while the tension between the reductionistic and nonreductionistic ideals among philosophers concerned with the unity of science is brought out nicely in Cat (2007); cf. also Batterman (2008).
- iv See for example Priestley (1796).
- v Assuming that Augustus de Morgan's (1872, 377) little verse is false:  
"Great fleas have little fleas upon their backs to bite 'em,  
And little fleas have lesser fleas, and so ad infinitum.  
And the great fleas themselves, in turn, have greater fleas to go on,  
While these again have greater still, and greater still, and so on."
- vi Cf. also Vemulapalli 2006 for a variant on this view.
- vii See Newman (2006, 2010), Jackson (2008) and Strogatz (2003) for a popular treatment.