CHAPTER 1

INTRODUCTION

The Invisibility of Chemistry

DAVIS BAIRD
South Carolina Honors College, University of South Carolina

ERIC SCERRI
Department of Chemistry and Biochemistry, University of California, Los Angeles

LEE MCINTYRE
Center for Philosophy and History of Science, Boston University

BUT *WHAT ARE* ALL THOSE CHEMISTS DOING?

Recently, one of us (Davis Baird) attended a meeting of historians of science and technology spanning all of the natural sciences and engineering and all (western) periods, ancient through contemporary. In the discussion of a paper on state-of-the-art history of modern (18th century forward) chemistry, a member of the audience made the claim that there was very little left to do in contemporary chemistry and that chemistry departments in his country were having trouble attracting graduate students. Baird found this perspective on contemporary chemistry both remarkable and implausible, and said as much. At the University of South Carolina (USC)—where he teaches—chemistry enrolls, and graduates, five times as many graduate students as physics. In this, USC is not unique.

The discipline of chemistry is, in fact, enormous and enormously productive. Joachim Schummer in this volume (Chapter 2) makes the point persuasively and concisely with data on the number of publications in various fields. With a grand total just shy of 900,000 papers indexed in chemical abstracts for the year 2000, chemistry is larger than all of the other natural sciences combined. After Baird suggested to the collected historians in the audience that contemporary chemistry was, in fact, a very active and productive discipline, a historian of mathematics sitting next to him leaned over and skeptically inquired, “But *what are* all those graduate students doing?”

“Making, measuring, and modeling . . . ” is how Baird’s colleague Catherine Murphy (Chemistry and Biochemistry, USC) would have replied. Recently, she and those in her lab have been making nanorods of silver with precisely controlled, diameters and lengths (Murphy and Jana 2002). It turns out that the aspect ratio (length/diameter) has a dramatic effect on the color of solutions of these rods. Short rods (20 nm by 30 nm) are orange, medium-length rods (20 nm by 100 nm) are red,

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and long rods (20 by 200) are blue.[1] Beyond the intrinsic scientific interest, various applications lie down the road. She also works on how strands of DNA flex, an important feature of how this long linear molecule wraps itself up into a tiny bundle for "storage" and unwraps when "being read."

Both research projects require each of her triumvirate: making, measuring, and modeling. Murphy has to *make*—synthesize—her nanorods, a multi-step process that will remind non-chemist readers of undergraduate chemistry labs carefully controlling temperature, pH, solution concentrations, reaction times, etc. The synthesized rods have to be *measured*—"characterized"—and here Murphy leans heavily on USC's Electron Microscopy Lab. Now she has rods of known aspect ratios, she knows how various properties—such as color in solution—depend on index ratios. But why? Here *models* for how the index ratio of the rods affects the absorption of radiation are necessary.

One cannot help but be struck by the ubiquity of chemistry. Everything in sight has the chemist's art written into it. Paints, varnishes, and other finishes all are the products of chemistry, some long established and (in this sense) "low tech," some new "high tech" paints with nanoparticles for striking visual and other functional qualities. There are batteries, light bulbs—reminding us of Oliver Sacks' recent "memoir of a chemical childhood," *Uncle Tungsten* (Sacks' uncle made better light bulbs through chemistry)—and liquid crystal computer displays. There is even chemistry hidden inside silicon chips, which are made by using ultra-precise lithography. Many of us use cheap "gel writer" pens with their new improved ink. And, of course, everywhere one looks, one sees plastics. In the 1960s film "The Graduate," Dustin Hoffmann was given this advice about the future—"one word, plastics." In this new century, that word might be "nanomaterials." Either way, it is chemistry.

Like the air we breathe, chemistry engulfs us. And like air, we take chemistry for granted. We do not see all of the making, measuring, and modeling that went into the world we inhabit. What are all those chemists doing, indeed! Yet somehow, despite its omnipresence, chemistry has remained largely invisible, denigrated by the physicist and, until recently, ignored by the philosopher. By way of an introduction to this volume, we briefly consider several of the more important reasons for chemistry's relative obscurity, and how the recent flourishing of work in the philosophy of chemistry—some documented in this volume—is helping to make this science more visible and accepted as an apt subject for critical reflection both within the laboratory and without.[2]

THEORETICAL ESCAPE FROM OUR MATERIAL BONDS

Until the last decade or so, historians, and especially philosophers, tended to focus on grand unifying theoretical visions instead of complicated local sights. Physics offers grand theories, and reflections on relativity, quantum theory, and physical theory generally have dominated 20th century philosophy of science. Chemistry offers a multiplicity of models drawing on both physical theory and experimental generalizations, each where appropriate. Yes, there is the periodic system, and we will see Ray Hefferlin's pursuit of a periodic system of molecules in this volume (Chapter 12). Joseph Earley (Chapter 11) discusses ways in which group theory can move chemical theory ahead, and Jack Woodyard (Chapter 13) develops a radically new way of interpreting quantum theory. However, much of the life of theoretical chemistry is better described by Murphy's "modeling," circumscribed attempts to make sense of synthesized local phenomena.

Theory, a philosophically acceptable substitute for fiction, like fiction, takes us away from the actual material world, away from the work-a-day world of the experimental chemist. There is a long tradition in philosophy that has tried to deny our clay-footed nature to see in us—and in our world—a more "important," more "fundamental," immaterial something, perhaps a soul and/or a set of first principles. Plato's peculiar ontological inversion, where the material world is, but an imperfect copy of such a realm of ideas, spells trouble for the philosophy of chemistry. Seeing chemistry—philosophically seeing chemistry—is perhaps like seeing our mortality. Denial is an enormously effective strategy.

Philosophers in denial have ample resources to draw on. Chemistry does sit right next to physics, with all its lovely unifying and foundational theory. Squinting our eyes up tight, it is possible to see chemistry as complicated applied physics. Even in denial, we say we are materialists, but the material world of our denial is the foundational world of physical theory, and so chemistry—in principle anyway—must be reducible to physics. But this has never been much more than an article of faith. The arguments for it have all relied on a highly sanitized picture of chemistry. It has been enough to persuade philosophers in denial that if one wants to understand science, it would be enough to understand physics. (To be fair, there is now a large group of philosophers who are not in denial, and many have pursued the philosophy of biology particularly vigorously. While there is also now a good group of philosophers of chemistry—several represented in this volume—this field has only very slowly, and recently, come to be accepted as part of the canon of philosophy of science.) However, we must be clear here: to understand science, it was often enough to understand physical theory. Through this work, we might gain some insight into chemical models and modeling, but the two other legs of Murphy's chemical tripod, making and measuring, are lost. Nonetheless, questions about the relations between chemistry and physics are central to understanding chemistry and chemistry's invisibility.

MAKING CHEMISTRY VISIBLE

A central aim of this volume is to continue to make chemistry more philosophically visible. Great strides already have been made in this and these are nicely documented in Schummer's contribution to this volume. Yet experience among the historians of science and technology suggests that more work is needed. Some of the fundamental sources for chemistry's invisibility can be found in the issues we have just quickly considered:

(i) the materiality of chemistry's objects;
(ii) the centrality and means of conceptualizing this materiality;
(iii) the nature and place of theory, and foundational issues in chemistry;
(iv) chemistry's relation to physics.

In reverse order, these issues establish the bases for the last four sections of the book:

Section 4, Chemistry and Physics;
Section 5, Chemical Theory and Foundational Questions;
Section 6, Chemistry and its Tools of Representation;
Section 7, Chemistry and Ontology.

Prior to these four sections are three more sections that mutually situate chemistry, the philosophy of chemistry, and the history and philosophy of science:

Section 1, Chemistry and the Philosophy of Chemistry;
Section 2, Chemistry and the History, and Philosophy of Science;
Section 3, Chemistry and Current Philosophy of Science.

Together, these seven sections take on chemistry's invisibility and make it—chemistry—more visible. We continue this introduction by briefly summarizing the work of the 18 authors of these seven sections.

CHEMISTRY AND THE PHILOSOPHY OF CHEMISTRY

Our first task is to situate the philosophy of chemistry. Joachim Schummer takes a more optimistic stance than our opening, but still he is struck by the failure until recently of philosophers to attend to chemistry. Given, chemistry's size, importance, and long and fascinating history, this fact cannot be ignored. It cries for explanation. Schummer provides excellent insight into the disciplinary forces that have driven philosophers' attention from chemistry. Indeed, remarkably, there is an inverse correlation between the amount of attention paid by philosophers to a field of study and the size of that field of study. Philosophers pay the most attention to their own history—which has the smallest literature—and the least attention to chemistry, which has the largest literature.

Schummer beautifully and concisely moves through the past, present, and future of the philosophy of chemistry. While there has been neglect in the past, the neglect has not been total. There has been a Marxist tradition of examining chemistry, vigorously pursued by Friedrich Engels, and carried on in Marxist countries. And, where philosophers have left the field vacant, chemists, chemical educators, and some historians of chemistry have moved to occupy it. There have been philosophical treatises on chemistry. Two important such contributions are considered in this volume, Aristotle—by Paul Needham (Chapter 3)—and Kant—by Jaap van Brakel (Chapter 4). Such was the not-completely neglected state of the philosophy of chemistry through the 1980s. There were important—but isolated—contributions, no sustained discussion of the subject, and no recognition by philosophers of science of the importance of the subject.

The situation began to change in the 1990s. This decade saw numerous conferences devoted exclusively to the philosophy of chemistry, the formation of two journals—*Hyle* and *Foundations of Chemistry*[3]—and the creation of the International Society for the Philosophy of Chemistry (ISPC). The ISPC has held annual international conferences on the philosophy of chemistry each summer, since 1997.[4] Indeed, several papers presented at the third, 1999, conference, held at the USC, form the basis for this volume.

Schummer outlines the spectrum of work that has made up this flourishing of the philosophy of chemistry. Reductionism has been a central issue (see Chapters 9 and 10, by Robin Hendry and G. K. Vemulapalli, respectively, in this volume). Also central are attempts to develop and adapt established concepts from the philosophy of science for chemistry—among others, naturalism, explanation, professional ethics, and themata in the history of science (see Chapters 5–8, by Otto Ted Benfey, Eric Scerri, Johannes Hunger, and Jeffrey Kovac, respectively). Philosophers have pursued conceptual analyses of key chemical concepts such as element, pure substance, compound, affinity (see Chapter 17, by Nalini Bhushan on natural kinds, and Chapter 18, by Michael Weisberg on pure substance).

Schummer closes his contribution speculating about, how philosophy of chemistry should develop. He suggests a variety of avenues of inquiry: What is the logic of chemical relations? What does the chemical system of classification (of chemistry's more than 20,000,000 known substances) tell us about ontology? What methods of discovery are peculiar to chemists, and how have they been so successful? How should we recast the relationship between science and technology in light of the long-standing history of the chemical industry and its close ties to academic chemistry? Here, we mention only a few of Schummer's suggestions. His entire list provides an exciting and compelling program for a fully developed mature philosophy of chemistry, one that rightly will force philosophy to rethink itself (see also Chapter 19, by Alfred Nordmann).

CHEMISTRY AND THE HISTORY AND PHILOSOPHY OF SCIENCE

The two contributions in the next section of the volume take up two important contributions to chemistry's relationship to the history and philosophy of science. First is Paul Needham's careful discussion of Aristotle's views about chemical reaction and chemical substance (Chapter 3). This is followed by Jaap van Brakel's eye-opening discussion of Kant's long neglected *Opus Postumum*, a work that only recently has come to wide attention. Its neglect allowed Kant's earlier dismissive views of chemistry to dominate philosophical considerations of chemistry. Here is a central source of chemistry's philosophical invisibility.

Atomism's rise, thanks to Dalton's resurrection of some ancient ideas of Democritus and Leucippus, has made atomists of all of us. However, Paul Needham (Chapter 3) makes clear that this conversion has been neither complete nor uncontested. Alternative approaches, most especially Aristotle's, remain embedded in contemporary chemical theory. Perhaps, the central theoretical problem that chemistry poses concerns combination: two distinct substances can combine to form a third yet distinct substance. Why does this happen? How does it happen? And, what does this say about how we conceptualize a substance's identity and properties? The atomists appear to have neat answers to these questions framed in terms of the combinations of individual indestructible atoms. However, Needham's more careful analysis shows, both how this approach is incomplete and how Aristotle's long ago criticisms of it have been important in the development of modern chemistry. Of particular interest here is how modal properties are used. Aristotle was more careful to recognize and deal with the manner in which the properties of elements in isolation are "lost," when in combination. However, since analysis can "bring them back," they must remain as a kind of potentiality. Here is one of several important features of Aristotle's theory that survives in modern chemistry (see Chapter 19, by Alfred Nordmann).

In his *Metaphysical Foundations of Natural Science*, Kant tells us that, "... chemistry can become nothing more than a systematic art or experimental doctrine, but never science proper; for the principles of chemistry are merely empirical and admit of no presentation a priori in intuition" (see Chapter 4, by Jaap van Brakel, for full quotation and references). Such was Kant's critical—and we use this word in both its common and its "Kantian" senses—assessment of chemistry. And this assessment, van Brakel shows us, has had an enormous impact. Even as late as 1949, the physicist and philosopher of science Herbert Dingle tells us that chemistry should not figure at all in the philosophy of science.[5] From Kant's critical point of view, chemistry suffered from two interconnected problems, it was insufficiently mathematical and its laws could only be found empirically, and hence these laws would always be subject to Humean skepticism. However, Kant's views on chemistry evolved in his post-critical period. Kant was specifically concerned with how his critical work had not come to terms with the diversity of substances chemists bring to our awareness and how his own metaphysical concept of matter did not deal well with this diversity (cf. Needham on Aristotle). This was a central project of Kant's *Opus Postumum.* Unfortunately, this work was first published—in a chaotic and unedited form—a century after Kant's death in 1804. The first English translation was published in 1993. Yet this is where Kant, in full awareness of the revolutionary developments and controversies that chemistry was undergoing at Lavoisier's hands and in the years following, begins to come to grips with chemistry as (at least an improper) science.

CHEMISTRY AND CURRENT PHILOSOPHY OF SCIENCE

The four contributions in the next section take up different long-standing concerns in the philosophy of science and look at them through the lens of chemistry. Although perhaps less frequently discussed in recent years, understanding how concepts play a central role in the historical development of science has much exercised philosophers of science. Otto T. (Ted) Benfey takes up this issue with work that develops Gerald Holton's notion of the role of themata in the history of science (Holton 1988). Eric

Scerri follows with a discussion of the role that reflections on chemistry can play in gaining deeper insight into the normative/descriptive distinction in the philosophy of science. Johannes Hunger shows how traditional concepts of explanation fail when transplanted to chemistry. And finally, Jeffrey Kovac develops an outline of an approach to professional ethics for chemists.

Holton is well known for arguing that general conceptual preferences—for example, for continuous theories or for theories that are symmetric in time—play an important role, over and above empirical data, in the historical development of science. Ted Benfey pursues this idea and develops a triad of opposing concept-pairs that provides a useful conceptual tool for looking at the history of science, and chemistry in particular. His three pairs are these: (1) reversible time–irreversible time; (2) continuity–discontinuity; (3) inner structure–outer structure. He illustrates how these six concepts work with numerous examples, many, although not all, taken from the history of chemistry. Thus, the ideal gas law posits an essentially uniform (or continuous) collection of point-mass (disregarding any inner structure) particles (reversibly) in motion. The theory works well, but not perfectly, and its imperfections can be traced to contraries of the three concepts employed. In fact, the particles are not point masses, but occupy space and have internal structure. They do not behave in a uniform manner at low temperatures, but will aggregate and exhibit discontinuities. And, of course, fundamental puzzles come from entropy and the irreversibility of time. With his three concept-pairs in hand, Benfey shows how fundamentally different traditions in science tend to focus on particular preferred collections of them. The mechanical sciences, which characterized the scientific revolution, tended to emphasize reversible time, a lack of inner structure, and discontinuity. The "organicist" (or "minority report" to the scientific revolution) emphasizes the opposites, directional time, inner structure, and continuity. And more generally, many scientific struggles have been struggles over how to incorporate these conflicting concepts.

Philosophy of science has long struggled to understand its position relative to the sciences. Is philosophy fundamentally about the—a priori—logic of science, dictating to scientists from epistemological foundations what can and cannot be an appropriate method? Or rather does philosophy fundamentally draw lessons about what are appropriate methods by observing how successful science goes about its business? We find more normative, a priori approaches in Kant, Frege and the logical positivists of the 20th century, and more descriptive, a posteriori approaches in Whewell, Mill and the recent "naturalist turn." Eric Scerri (Chapter 6) reminds us of this history and then presents a bit of his own history of coming to terms with chemical orbitals. Quantum mechanics tells us that orbitals do not exist, and early on Scerri drew strong normative conclusions from this, urging chemists from his stance in the foundations of chemistry, to recognize that these chemical workhorses were fictions. Chemists were not moved. And Scerri began to reconsider the strength of his normative position. He has arrived at a kind of compromise that draws on chemist Fritz Paneth's understanding that chemistry must at once recognize that quantum theory lies at chemistry's base, while also remaining an autonomous science that uses concepts such as orbitals and other even higher level macroscopic concepts. Scerri shows us how the philosophy of chemistry can teach the philosophy of science to be both descriptive and normative. Both attitudes—a term Scerri consciously takes from Arthur Fine—are important to our philosophical work and indeed to the work of practicing scientists.

Johannes Hunger (Chapter 7) takes on another of the standard topics in the philosophy of science, explanation. Hunger examines, in detail, various ways that chemists explain and predict the structural properties of molecules. We learn about ab initio methods, empirical force field models and neural network models, each of which have been used to explain and predict molecular structure. And we learn that none of these approaches can be subsumed under either hypothetico-deductive or causal models of explanation. Either chemistry does not offer proper explanations (the normative option) or our philosophical models for explanation are inadequate to cover explanation in chemistry (the descriptive option). Hunger takes the descriptive option and sketches a more pragmatic approach to the explanation that develops Bas van Fraassen's approach to explanation for chemistry. Once again, we find that the philosophy of science has much to learn from the philosophy of chemistry.

This section closes with a sharply normative chapter written by a chemist on professional ethics. Jeffrey Kovac argues that ethics lies at the very heart of chemistry, and science more generally. As an institution that grows our knowledge, science depends on the good moral character of its practitioners. Kovac has made good on these views in practice, incorporating ethics into his chemistry curriculum. Here (in Chapter 8), he outlines his approach to ethics for the sciences. He draws on the fact that the sciences are professions, and as professions, they depend on internal agreements among their practitioners to behave according to certain standards, and external agreements with the society in which they are embedded to provide a certain kind of product in return for support and monopoly status as purveyors of scientific knowledge. Kovac draws on Robert Merton's four ideals of science to articulate the nature of the profession of science:

(i) Universalism—science aims at universal truth based on universally accepted criteria;
(ii) Communism—scientific knowledge is a public or community good;
(iii) Disinterestedness—the advancement of science is more important than the advancement of its practitioners;
(iv) Organized skepticism—claims to scientific knowledge are provisional, based on accessible data and subject to revision
(Merton 1973).

Kovac concludes his chapter sketching a moral ideal for science. He focuses on two attributes: (1) scientists who make up the profession of science must have the habit of truth. Honesty with oneself, with one's colleagues, and with the society one serves is essential to the flourishing of science; (2) scientific goods should be exchanged as gifts, not commodities. Gift exchange is tied to all of Merton's ideals, but most closely to communism; gifts are part of how a community of inquirers establishes and preserves itself.

CHEMISTRY AND PHYSICS

The two chapters in the next section take up chemistry's relation to physics and, in particular, the bug-a-boo of reductionism. The chapters complement each other. The first, by Robin Hendry, looks at chemistry's relation to physics from the point of view of philosophy, bringing the careful analyst's conceptual scalpel to the minefield of reductionism and emergentism. The second, by G.K. Vemulapalli, looks at chemistry's relation to physics from the point of view of chemistry, simultaneously acknowledging the importance of the fundamental laws of physics for chemistry, while conceding none of chemistry's autonomy.

It is relatively easy to talk and gesture about how chemistry either does or does not reduce to physics. It is much harder to spell out exactly what is required to make good on the claim that chemistry does (or does not) reduce to physics. Philosophers have a concept of supervenience. In the case we are focused on here—chemistry putatively reducing to physics—supervenience requires that every chemical change be accompanied by a physical change. This is nearly universally held, for example, if two molecules are identical in all physical respects, they will not differ chemically. However, supervenience is not sufficient for the reduction of chemistry to physics. There could be "downward causation," where it is the chemical facts and laws that drive the physical facts and laws, not the other way around. Robin Hendry (Chapter 9) argues that those committed to the reducibility of chemistry to physics have not ruled out the possibility of downward causation, and moreover, he presents substantial evidence from the manner in which quantum mechanical descriptions for molecules are constructed and deployed by chemists in favor of downward causation. Quantum mechanical descriptions of molecules that have explanatory and descriptive power are constructed from chemical—not physical—considerations and evidence. Here in precise terms, we see chemistry supervenient on physics, but still autonomous, not reducible to physics.

So, if chemistry is not reducible to physics, what is the relationship between the two disciplines? This is the question that G.K. Vemulapalli takes up in Chapter 10. Drawing on a wealth of experience in the practice of chemistry, Vemulapalli looks at how chemists use physical theories, how they develop chemical theories over and above physical theories, and how these two theoretical domains relate to each other. It is clear from many examples that developments in physics profoundly influence chemistry. Relative molar masses—one of several examples that Vemulapalli presents—are now routinely measured by mass spectrometry working in combination with the ideal gas law. It is also clear from many examples that developments in chemistry influence physics. Faraday's work as an electrochemist led to Stoney's introduction of the concept of the electron, and Nernst's study of low temperature equilibria led to the third-law of thermodynamics. The development of quantum theory has played a major role in the chemical understanding of bonds. However, and here is one of Vemulapalli's main points, chemists do not *and cannot* simply plug chemical situations into the Schrödinger equation and get useful results. They must augment straight physical theory with chemical concepts, bond energies and bond lengths, for example. As Vemulapalli puts it, physical law provides fundamental conceptual insight and boundary conditions on what is possible, chemists have to add to this to find out how actual chemical species behave.

CHEMICAL THEORY AND FOUNDATIONAL QUESTIONS

Hendry and Vemulapalli nicely frame the space for the work taken up in the next section. Fundamental physical theories such as quantum mechanics raise difficult foundational questions that have demanded the efforts of many powerful minds in physics and the philosophy of physics. As chemistry is not reducible to physics, there is an autonomous space for chemical theory and for foundational issues in chemical theory. Three such issues are raised in this section. Joseph Earley examines the role of symmetry in chemistry and argues for closer attention to group theory on the part of his fellow chemists. Ray Hefferlin seeks to extend the idea of a periodic law from elements to compounds. Jack Woodyard takes on the fundamental obstacles that get in the way of a more straightforward application of quantum theory to molecules.

Joseph Earley (Chapter 11) argues for the importance of group theory both in chemistry and in the philosophy of chemistry. He shows how group theoretical concepts can shed needed light on several fundamental problems in chemistry. For one, there is the problem of chemical combination that we have already seen (Chapters 3 and 4, by Paul Needham and Jaap van Brakel, respectively). For another, there is the problem of reduction and emergence that we also have seen (Chapters 6, 9, and 10, Eric Scerri, Robin Hendry, and G.K. Vemulapalli, respectively). Earley looks at philosophical contributions to mereology (the study of parts and wholes). He shows that mereology, as it is currently developed, is incapable of dealing with chemical combinations, for, in general, the properties of elements alone are significantly changed when in combination. Earley suggests that group theory, and in particular the concept of closure under the group operation, provides the necessary conceptual apparatus to move mereology ahead, so that it can deal with chemical combination. Earley also suggests that group theory is exactly what is needed to provide a conceptually sharp way of articulating how a more complex system can emerge from a simpler system, while remaining supervenient on the simpler system—exactly the situation that Hendry discusses with respect to chemistry and physics.

Dimitri Ivanovich Mendeleev's periodic table of the elements has been tremendously important in chemistry and the philosophy of chemistry. It provides a powerful organizing principle that has led to the discoveries of new unsuspected elements and, until recently, it stands as one of the best examples of a genuinely chemical law. There have been—not completely successful—attempts to explain the periodic law with quantum theory (Scerri 2003b), but it remains, like Darwin's theory of natural selection in biology, a cornerstone of chemistry. It would be spectacular if a similar periodic system could be developed for molecules. It would help organizing the massive complexity that constitutes the huge number of known chemical species, and it would help predict new compounds that might be synthesized and developed for practical purposes. It would also be a wonderful further example of chemistry's autonomy. Ray Hefferlin (Chapter 12) has been a main player in two decades of attempts to develop such a system of molecules. Here, he provides an overview of the history of these attempts, their problems, and their prospects.

In our last chapter on the theoretical and foundational issues in chemistry (Chapter 13), Jack Woodyard constructively attacks the way classical quantum theory is fudged in quantum chemistry. Woodyard argues for fundamental change, abandoning Hilbert space representations in favor of a complex three-dimensional space in which "matter-waves" interact. We have already seen that the application of quantum theory to chemistry is not straightforward and requires additional input from experimental data and from techniques of approximation that work, but which cannot be motivated on theoretical grounds (Chapters 6, 7, 9, and 10, by Eric Scerri, Johannes Hunger, Robin Hendry, and G.K. Vemulapalli, respectively). Woodyard presents additional evidence that this traditional approach only works through the use of numerous band-aids to cover over assumptions that are known to be mistaken. The theory provides no means that is not *ad hoc* to visualize molecules, and perhaps most damning, as more terms are calculated in the theoretical series, the results move further from experimental values. Woodyard offers an alternative theory that retains the fundamentally correct core of quantum theory, but develops it as a theory of matter-waves in three-dimensional space, and he shows that his alternative provides results that agree with experiment better than the standard approach. Woodyard is aware that fundamental change, such as that which he offers, is almost never smoothly adopted, replacing current dogma, and he offers some engaging insights into revolutionary science from his point of view as a revolutionary.

CHEMISTRY AND ITS TOOLS OF REPRESENTATION

These issues about chemical theory and its relation to physical theory are central to the philosophy of chemistry, but they do not encompass the whole field. How chemistry goes about representing its objects is extremely important, both to the conduct of chemistry and to our philosophical understanding of chemistry. This section includes three chapters on chemistry's tools of representation. In the first, Ann Johnson describes the introduction of computers into chemical engineering. This is important because the rise of computer-aided design radically—incommensurately—changed the field. Johnson's contribution also is important because she reminds us that the philosophy of chemistry cannot ignore its technological end, chemical engineering. In the next chapter, Sara Vollmer considers seemingly simpler tools, the ways in which we symbolize chemical species "on paper." Her discussion probes the differences between pictorial representations and linguistic ones. Finally, the philosopher/chemist pair, Daniel Rothbart and John Schreifels, examines the pre-suppositions that go into the design of analytical instruments.

Ann Johnson's story about the introduction of computers into the practice of chemical engineering (Chapter 14) reminds us of several important features about science. Tools make a difference. Furthermore, it is through communities of practitioners that tools are introduced and these communities bring specific problems—indeed as Johnson has it, they are defined by their problems—to their work. By the end of the story, chemical engineering c. 1990, the work done by a chemical engineer has changed radically from that done c. 1950. Some changes might be expected (although, perhaps only in hindsight). Much chemical engineering involves working with partial differential equations. Prior to computers, which can iteratively produce numerical approximations, a chemical engineer had to work with analytically soluble equations. Computers relax this constraint, but, of course, they produce their own constraints. Initially, specialist programmers were necessary. This produced a disciplinary problem, which over time was solved by incorporating computer programing into the training of chemical engineers. When first introduced, computers were used to crunch numbers, while the surrounding engineering practice stayed more or less the same. However, as the possibilities of the tool became better understood, the practice itself changed. The computer was developed to simulate operations, and this opened up (and simultaneously closed off) a whole new field of operations for chemical engineers. In the end, the kinds of problems, acceptable solutions, necessary training, day-to-day practices, and disciplinary setting of chemical engineering all changed, producing a kind of incommensurability that stories of theory change miss.

Sara Vollmer's contribution (Chapter 15) concerns what seems a much simpler chemical tool, the manner in which we symbolize chemical species on paper. She contrasts John Dalton's approach with Jakob Berzelius's approach. Berzelius developed a forerunner to the now-common "H_2O" representation where compounds are represented in terms of the relative molar numbers of their elemental constituents. Dalton's approach was more pictorial. Sulfur trioxide (Dalton's understanding of sulfuric acid) was shown as a central circle (with some conventional markings to indicate its being sulfur) surrounded by three other "oxygen" circles, an approach that presages various "ball-and-stick" representations used today. Vollmer's interest here is to tease out how pictorial representations, such as Dalton's, differ from Berzelius's more linguistic representations. The answer lies somewhere in the geometry that the representation shares with its object, although, particularly when it comes to the illusion of three dimensions on a two-dimensional surface, this answer requires considerable care to explicate.

The final chapter in this section brings together Johnson's concerns with instrumentation and how communities interact with instrumentation, and Vollmer's concerns with pictorial representation. Daniel Rothbart and John Schreifels (Chapter 16) discuss a variety of instruments, from Hooke's microscopes to Binnig and Rohrer's scanning tunneling microscope. They are concerned to show that instruments are not passive "transparent" devices that merely "open a window" on a part of the world that is otherwise inaccessible. Instruments are active devices and in multiple senses. Instruments must be made, and this means that we have to rely on the extant collection of materials and techniques to work them. However, even before we put hand to lathe we have to design, and here Rothbart and Schreifels's add to Vollmer's discussion of pictorial representation. Rothbart and Schreifels think of instrument designs as thought experiments, where one can, through reading the diagrams, think through how the instrument will interact with its specimen. This reminds us that the passage through an instrument from specimen to observation is anything but passive. Instruments probe specimens generate a signal and modify this signal, all along the path to creating information about the specimen. Rothbart and Schreifels argue that it is in virtue of the mechanical operations that instruments and nature share, that we can trust what we learn from instruments. They draw both an epistemological moral—only instruments that properly share their modes of operation with their objects will produce genuine knowledge—and an ontological moral—the operations of the world are of the same sort as the operations of instruments. Speaking of "a clockwork universe" is more than mere analogy.

CHEMISTRY AND ONTOLOGY

Rothbart and Schreifel's ontological speculations bring us to the last section of the book, where we find chemistry's most profound lessons, ontology. All three chapters, here, deal with the lessons chemistry has for our understanding of substance. And, as Michael Weisberg reminds us, chemistry is the science of the structure and reactivity of substances. So, there is no surprise that there is much to be learned here. The first two chapters—Chapters 17 and 18, by Nalini Bhushan and Michael Weisberg—are about chemistry's lessons about natural kinds. In the philosophical literature, written by philosophers with at best a superficial knowledge of chemistry, chemistry is frequently cited as a bountiful source of paradigm natural kinds. Is not water H_2O, after all? Bhushan and, separately, Weisberg bring more chemical sophistication and skepticism to this simplistic notion of natural kinds. Water is not (simply) H_2O. Alfred Nordmann, in Chapter 19, draws on the work of Émile Meyerson and Gaston Bachelard—two philosophers with some genuine chemical knowledge—to articulate a more general, a richer, and a metachemical notion of substance. This metachemical notion of substance improves upon the metaphysical notion that has been plaguing us with philosophical pseudoproblems for centuries.

Nalini Bhushan argues that chemical kinds are not natural kinds. They are not natural kinds because many chemical kinds are human-crafted—synthesized—kinds and do not occur "naturally." However, they are also not natural kinds in the more important sense that chemistry does not offer a univocal way of carving up substances (synthesized or "natural") into kind categories. How a chemist classifies kinds, has to do with local chemical and functional needs, and is responsive to these needs. For some purposes, having a particular kind of reactivity will drive classification; for other purposes, structural issues will drive classification; and for yet other purposes, other classifications are appropriate.

Michael Weisberg's water example (Chapter 18) helps to make this point. "Ordinary," although purified (but how purified?), water found "naturally" on the Earth contains typical, percentage-wise predicable isotopic isomers. While most water is composed of "ordinary" "one proton–one electron" hydrogen, a small percentage is composed of a heavier isotopic isomer of hydrogen—"one proton–*one neutron*–one electron," "deuterium," or "D." We symbolize "heavy water," HDO, instead of H_2O. For many purposes, the water we want to talk about *must* contain the standard percentages of ordinary H_2O *and* "heavy" HDO. Properties such as freezing point and viscosity depend on this "water natural kind" having the "naturally occurring" percentages of isotopic isomers. Sometimes, it is crucial to draw distinctions between these isotopic isomers—and to separate them in the lab, preparing isotopically pure samples of the various "kinds" of water. Heavy water is used as a moderator in some nuclear reactors, but you would not want to drink it.

Bhushan and Weisberg both take pains to point out how chemical kinds are more complicated than philosophers untutored in chemistry might think (or wish). They take these facts from chemistry in slightly different directions. Bhushan argues that the realist conclusions that chemically naïve natural kind talk engenders are not supported by genuine chemistry. Instead, she opts for a more situated "particularist" approach to chemical kinds that takes from Nancy Cartwright's ontological views (Cartwright 1994, 1999). The position is realist, and the chemical kinds employed are "really out there," but only in locally constructed—perhaps synthesized—ways, not theoretically globally. Weisberg argues that work in the philosophy of language that causally ties reference to essences identified in an initial act of dubbing (Kripke 1980; Putnam 1975) rests on a false assumption. This assumption is what Weisberg calls the "coordination principle," and it asserts that ordinary kind talk (e.g., "water") can be mapped onto scientific kind talk (e.g., H_2O), where we actually discover the nature of these essences. However, as we have seen, water is not H_2O, and the coordination principle cannot be true. Weisberg urges us to consider a better coordination principle that allows references such as "water" to be responsive to the context of use. When a guest asks for a glass of water, it is the ordinary bulk liquid with its standard percentages of isotopic isomers that (no doubt, usually unconsciously, or even "metaphysically") "water" refers to. When a nuclear engineer asks for the valve for the water moderator to be opened, "water" refers to "heavy water."

So, chemistry teaches us that kinds are more complicated than we thought. Alfred Nordmann (Chapter 19) takes this conclusion further, the very notion of substance is more complicated than we thought. Our "metaphysical" notion of substance focuses exclusively on the millennially old "problem of change": what stays the same through change? However, to understand the material world we inhabit, we need a richer notion of substance, a notion that is sensitive to how substances come into being, how we identify them as substances, and how we project them forward into a world constantly in the making. Metachemistry gives us this notion of substance. While not denying the metaphysical notion of substance, metachemistry provides a broader notion that embraces the metaphysical "sub-stratum" notion, but adds important elements to it. Nordmann describes Bachelard's trio: "sub-stance"—that which lies behind observable phenomena; "sur-stance"—that which emerges in our engaging the material world; "ex-stance"—that excess of meaning that substance concepts have, and which allow us to project these substances beyond their context of creation. Nordmann connects this work by Bachelard with more recent work by Bruno Latour, where the focus is on the work scientists perform to bring substances into being. He also connects it to Peirce's notion that the real is what is arrived at, at the end of inquiry. We may start with a purely metaphysical notion of substance, but we end with a real metachemical notion.

As one can see, even through this brief summary of the papers that are contained in this volume, the philosophy of chemistry is now well launched as a discipline. After predictable growing pains over the last few decades, we feel that the field is now mature enough to offer a quorum of good work, such that the subtitle of this volume—"Synthesis of a New Discipline"—may live up to its promise. This, of course, cannot be judged by the merits of any *a priori* argument over the need for a new discipline, but only by the content of the work that already exists in the field. It is to this that we direct the reader in the pages that follow.

NOTES

1. Many institutes have recently sprung up to study nanoscience, all having a strong contingent of chemists. For example at UCLA, the institution of another of the editors of this volume (Scerri), the California Nano Systems Institute (CNSI) has recently been founded following the award of a grant amounting to approximately $50 million.
2. Even in the realm of popular science books, chemistry appears to be under-represented with physics and biology claiming far greater shelf space. Some exceptions include books on the periodic table and books by Peter Atkins, Philip Ball, and Roald Hoffmann all of whom have made valiant efforts to popularize chemistry.
3. The websites for the two journals are http://www.hyle.org/index.html and http://www.kluweronline.com/issn/1386-4238, respectively.
4. Several earlier meetings were also held in Germany and the UK, including one at the London School of Economics, in March 1994 and the first International Summer School in Philosophy of Chemistry, in July 1994. (Scerri 2003a). A detailed survey of the history of the field has been published (Van Brakel, 1999) and several books on philosophy of chemistry have also appeared (Bhushan and Rosenfeld 2000; Schummer 1996; Van Brakel 2000).
5. Nevertheless, Dingle who founded the *British Journal for the Philosophy of Science* was sufficiently interested in chemistry to act as the co-editor of the philosophical essays by the chemist Fritz Paneth (Dingle and Martin 1964).

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