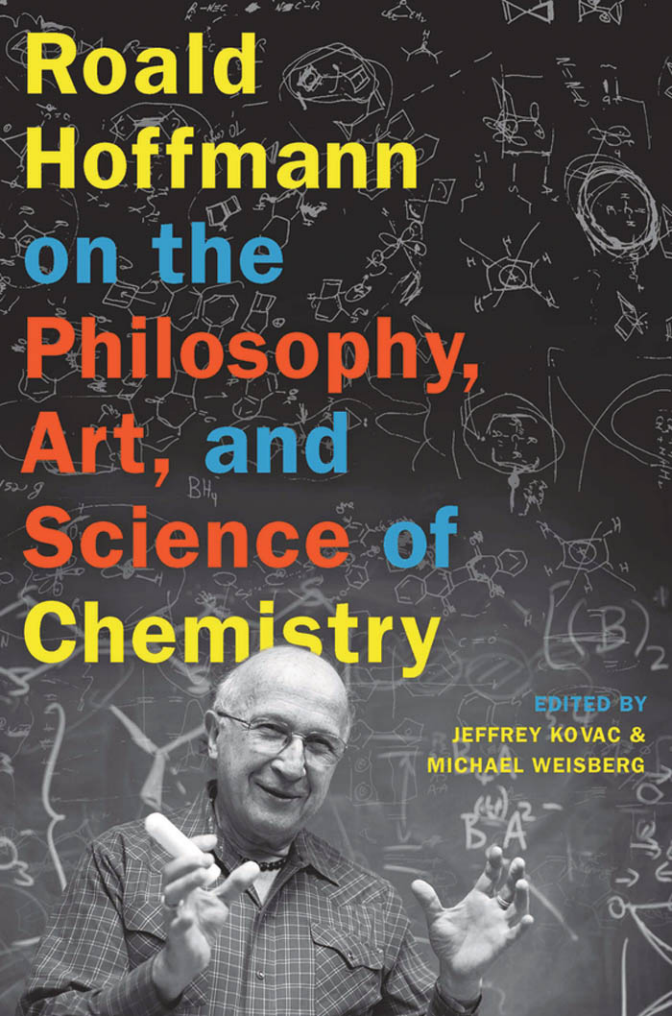
Roald Hoffmann on the Philosophy, Art, and Science of Chemistry



EDITED BY
JEFFREY KOVAC &
MICHAEL WEISBERG

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and

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From the Editors

Throughout the process of bringing this book to press, the editors have had the complete cooperation of Roald Hoffmann. To begin, Roald sent us copies of his papers with suggestions of what to include. Once the selection had been made, he revised each of the papers to eliminate unnecessary redundancies and to bring the scientific content and the references up to date. He also provided original figures. He has read many drafts of the introduction, providing suggestions for improvement but allowing us the intellectual freedom to introduce his work as we felt most appropriate. Without his help, this book would not have possible. Working with Roald has been both intellectually stimulating and personally rewarding.

From Jeffrey Kovac

I am grateful to my long-time administrative assistant, Rai-Lynne Broach Alexander, for her help in preparing the final manuscript. As always, the support and encouragement of my wife, Susan Davis Kovac, has been essential to the success of this project.

From Michael Weisberg

I would like to thank Simon Garcia and Deena Skolnick Weisberg for conversations and correspondence that greatly improved this project.

From Roald Hoffmann

It was Jeff Kovac's and Michael Weisberg's idea that it might be useful to bring out a collection of my philosophical, social, artistic, and educational writings, scattered as

they were across the literature. That it was necessary to do this is in a way testimony to my lack of ability to integrate these writings, the carving out of my own land twixt philosophy, chemistry, and poetry, into a coherent book. But more than that, the crafting of this assemblage is an act of friendship on the part of two fellow thinkers. We are on the same wavelength, so to say. Or the same wave, at least. I am very grateful to both for their work on the project.

At the end of chapter 1 I thank the people, so many of them, that have encouraged and supported me over the years. I would add here Catherine Kempf for research and help in editing the essays for this volume. Thank you all for helping me reflect.

Contents

Introduction xiii
MICHAEL WEISBERG AND JEFFREY KOVAC

1. Trying to Understand, Making Bonds 1
ROALD HOFFMANN

Part 1 CHEMICAL REASONING AND EXPLANATION

2. Why Buy That Theory? 15
ROALD HOFFMANN

3. What Might Philosophy of Science Look Like If Chemists Built It? 21
ROALD HOFFMANN

4. Unstable 39
ROALD HOFFMANN

5. Nearly Circular Reasoning 45
ROALD HOFFMANN

6. Ockham's Razor and Chemistry 53
ROALD HOFFMANN, VLADIMIR I. MINKIN, AND BARRY K. CARPENTER

7. Qualitative Thinking in the Age of Modern Computational Chemistry, or What Lionel Salem Knows 81
ROALD HOFFMANN

8. Narrative 88
ROALD HOFFMANN

9. Learning from Molecules in Distress 97
ROALD HOFFMANN AND HENNING HOPF

10. Why Think Up New Molecules? 114
ROALD HOFFMANN

11. Protean 120
ROALD HOFFMANN AND PIERRE LASZLO

12. How Should Chemists Think? 128
ROALD HOFFMANN

Part 2 WRITING AND COMMUNICATING IN CHEMISTRY

13. Under the Surface of the Chemical Article 145
ROALD HOFFMANN

14. Representation in Chemistry 163
ROALD HOFFMANN AND PIERRE LASZLO

15. The Say of Things 193
ROALD HOFFMANN AND PIERRE LASZLO

16. How Symbolic and Iconic Languages Bridge the Two Worlds of the Chemist: A Case Study from Contemporary Bioorganic Chemistry 222
EMILY R. GROSHOLZ AND ROALD HOFFMANN

17. How Nice to Be an Outsider 242
ROALD HOFFMANN

18. The Metaphor, Unchained 248

ROALD HOFFMANN

Part 3 ART AND SCIENCE

19. Art in Science? 255

ROALD HOFFMANN

20. Science and Crafts 261

ROALD HOFFMANN

21. Molecular Beauty 272

ROALD HOFFMANN

Part 4 CHEMICAL EDUCATION

22. Teach to Search 295

ROALD HOFFMANN

23. Some Heretical Thoughts on What Our Students Are Telling Us 311

ROALD HOFFMANN AND BRIAN P. COPPOLA

24. Specific Learning and Teaching Strategies That Work, and Why They Do So 319

ROALD HOFFMANN AND SAUNDRA Y. McGUIRE

Part 5 ETHICS IN SCIENCE

25. Mind the Shade 337

ROALD HOFFMANN

26. Science and Ethics: A Marriage of Necessity and Choice for This Millennium 339

ROALD HOFFMANN

27. Honesty to the Singular Object 347
ROALD HOFFMANN

28. The Material and Spiritual Rationales Are Inseparable 360
ROALD HOFFMANN

Sources 377
Index 379

Roald Hoffmann on the Philosophy, Art, and Science of Chemistry

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Introduction

MICHAEL WEISBERG AND JEFFREY KOVAC

Roald Hoffmann has been widely recognized for his fundamental research in chemistry, as well as for his literary career as a poet, playwright, and essayist. But Hoffmann is also a philosopher of science who has made significant contributions to our conceptual, historical, and normative understanding of chemistry. This book collects many of Hoffmann's philosophical essays, which represent a significant and unique understanding of chemistry and its broader context. It is divided thematically into five sections: Chemical Reasoning and Explanation, Writing and Communicating Science, Art and Science, Education, and Ethics.

Hoffmann characterizes his own scientific research as "applied theoretical chemistry." Reflecting on his own work in this area has led Hoffmann to consider the problem of explanation in chemistry. Hoffmann rejects a strictly reductionist framework in which the best explanation of a chemical phenomenon is always its underlying physical processes. While the methods of quantum chemistry are powerful tools for computing molecular properties, he argues that chemists need to provide explanations using chemical concepts. Hoffmann calls this explanatory practice *horizontal reasoning*.

Science is public knowledge and must be communicated both to the scientific community and to the general public. Not only has Hoffmann written extensively for both audiences, he has also made a study of scientific writing, both the form and the language. Perhaps uniquely among the sciences, the language of chemistry is pictorial and has what Hoffmann calls an "iconic vernacular." Hoffmann's reflection on the graphical presentation of chemistry has led him to a wider consideration of the relationship between art and chemistry, a connection made even stronger by the centuries-old craft tradition which is one of the sources of modern chemistry.

One of the ways that chemists communicate is as teachers. Hoffmann himself is a gifted and dedicated teacher who believes, quite correctly, that research and

teaching are intertwined. We have included several essays that discuss his insights into chemical education.

The final section of the book is a collection of essays and two unpublished lectures on ethics in science. Although many of Hoffmann's popular essays and his plays discuss ethical themes, we have chosen to include these essays because they take up ethical questions explicitly, focusing on the contemporary problem of environmental degradation. Hoffmann explores the paradoxical position of the chemical industry as a source of significant pollution but also a needed partner in solving environmental problems. He argues that *green chemistry* can and must play a central role in reducing environmental degradation.

Hoffmann is *reflective,* in a way that is relatively rare in chemistry. He thinks and writes about the way chemistry is practiced, how chemistry is embedded in society, and the psychology of its practitioners. He also writes in a direct and expressive manner, perhaps as a consequence of his writing career in poetry and theater. This book is a collection of his thinking about the molecular science.

Chemical Reasoning and Explanation

Throughout his writing on this subject, Hoffmann has argued that chemical reasoning and explanation have a distinct character. This is at odds with the classical tradition in philosophy of science that seeks a uniform logic for explanation and confirmation, largely based on paradigm episodes in the history of physics. Recent developments in philosophy of science have emphasized the extent to which biology deviates from these logical patterns. The essays in this section argue for a similar thesis and develop a theory about the form of chemical explanation across most areas of chemistry.

Hoffmann's account of chemical explanation begins from the recognition that the central chemical activity is the synthesis of molecules. Chemists make new molecules, some for practical applications, others because they are of theoretical interest, or just because they are a challenge. Although chemistry is a diverse field, encompassing many research activities, much of this activity is aimed at understanding molecular structures and transformations between these structures, in other words, chemical synthesis. To use Hoffmann's own expression, creation rather than discovery is the goal of much of the chemical community.

The key to understanding how chemists create molecules is found in the molecules' three-dimensional structure. One account of how scientific explanations work says that to understand this structure we need to show how it can be derived from the laws of physics. This covering law account of scientific explanation is what Hoffmann terms the "vertical" model of chemical explanation. Quantum theory allows the chemist to write down the molecular Hamiltonian and find an approximate solution for the molecule's wavefunction and the energy. This, in turn, allows for the prediction of molecular structure and other properties of the molecule.

With increasingly sophisticated mathematical techniques and ever faster computers, it is now possible to compute the properties of relatively large molecules this way. But do these calculations constitute a chemical explanation of molecular structure? According to the covering law account, with a few emendations to allow for approximations, they are paradigm cases of scientific explanations. However, Hoffmann argues that these are not explanations at all because they convey no chemical understanding, which is the kind of understanding needed by the experimentalist.

What is chemical understanding and why isn't it conveyed by quantum mechanical calculations? Hoffmann argues that chemical understanding arises when explanations deploy purely chemical concepts in a form that can be used across a range of similar situations. He calls such explanations "horizontal," because of the use of chemical, not physical, concepts. When the conformation of a chemical structure is explained by reference to a chemical property like steric hindrance, this gives the chemist an idea about what the structure of a similar, but distinct molecule would be. Further, horizontal explanations are contrastive. They don't just explain why p happened, but why p happened instead of q.

It is easy to see why contrastive explanations are important in chemistry. The key is chemical synthesis. To manipulate matter, one needs to know more than "quantum mechanics says that this bond angle is the most stable." Rather, one needs to be able to anticipate how the bond angle will change as a bulky protective group or a new substituent is added. There is thus a deep connection between identifying trends, contrastive explanations, and chemical synthesis.

Hoffmann's essays also point to another interesting feature of the chemical concepts used in chemical explanations. Such concepts, he argues, are often fuzzy, vaguely defined, and changing through time. Concepts such as acidity, electronegativity, aromaticity, and functional group involve vague predicates. While chemists can give definitions and accounts of them, most attempts to draw rigid boundaries around them have not been fruitful. Moreover, penetrating empirical observations and Gedanken experiments can take what seems like a straightforward definition, acidity as the concentration of H^+ in an aqueous solution, and show that this definition is inadequate. In the case of acidity, what should we say when water isn't the solvent? Or when other acceptors of electrons are present, but H^+ is not? Or when we are dealing with gases or solids instead of liquid solutions?

Chemical explanations and predictions often rely on analogical arguments, narrative, and stories. Why are chemical arguments developed this way instead of via exclusive appeals to mathematics? To answer this question, Hoffmann emphasizes the psychological needs of the intended audiences of chemical argumentation. He argues that since science is made by human beings, it must be understood in human terms, even insofar as it is aiming to tell us objectively about the world. As Hoffmann points out in the essay "Nearly Circular Reasoning," "Science is a curious mixture of the real and the ideal, the material and the spiritual, held together by discourse or

argument. The latter is sometimes mathematical, but more often it transpires in the words of some language. [. . .] Try to imagine a scientific article or seminar without the glue of words or argument."

Hoffmann's essays also address issues of confirmation and testing, in particular the overreliance on heuristics of simplicity. Many scientists accept as an axiom the doctrine known as Ockham's Razor: When two hypotheses explain a phenomenon equally well, one should choose the simpler hypothesis. Medieval theologian and philosopher William of Ockham applied the principle to ontological arguments, but chemists are more likely to appeal to it as a justification for favoring a simple reaction mechanism over a more complex one.

In their essay, "Ockham's Razor and Chemistry," Hoffmann and his collaborators, Vladimir I. Minkin and Barry K. Carpenter, look at the strengths and limitations of the use of the Razor in chemistry, particularly in the analysis of chemical reaction mechanisms. Agreeing with much of the philosophical literature, they point to the role of Ockham's Razor in curve fitting. They point out that even with highly correlated data, where a simple linear fit would be deemed appropriate, there are always many more nonlinear curves that will fit that collection of points. However, this nonlinear curve requires many more parameters, so allowing this possibility opens us up to what they call "real indeterministic chaos—the infinity of hypotheses that fit."

As in curve fitting, chemists are often drawn to the simplest mechanism, even when many other, more complex mechanisms cannot be ruled out. Although this view is often reasonable, Hoffmann, Minkin, and Carpenter argue for caution because nature is sometimes not as simple as we might hope. For example, a reaction can proceed through multiple paths depending on the circumstances. They also point to another consideration in the choice of reaction mechanism: future productivity. The more ornate hypothesis might be richer in its ability to lead to experiments that help us understand the phenomenon. Hoffmann and his collaborators conclude that we ought to look for simplicity, but be wary of it.

The final set of papers in this section concern the relationship between theory and experiment. In a science such as chemistry, where more than 95% of its practitioners are pure experimentalists, what is the proper role of the theorist? Hoffmann's view is that chemical theorists have a dual role in the chemical community: First and foremost, theorists should be explainers and should construct horizontal explanations. Second, Hoffmann believes that theorists should stimulate experiments. One way that they can do this is by imagining new molecules—interesting structures that are likely to be stable but have not yet been made.

Given that more than one hundred million structures have already been characterized by chemists, why would one want to imagine even more molecules? One motivation is to allow or encourage theorists to participate in the creative part of chemistry: synthesis. But a second and more important reason is to test fundamental ideas about molecular structure and properties. In this context, there is much to be learned from what Hoffmann calls "molecules in distress," structures that bend

the normal rules. For example, carbon prefers to form four bonds that are oriented in a tetrahedral arrangement. But molecules can be made, or imagined, where the bond angles are significantly distorted. One can learn much about molecular stability and reactivity by studying these structures. These distressed structures also present a significant challenge for the synthetic chemist. Can they actually be made? Finally, Hoffmann points out the sheer beauty and pleasure of this type of work. Humans love to play and inventing new things is one of the most delightful of intellectual games.

The study of distressed molecules raises a more general question about experimentation. Hoffmann believes that standard discussions of scientific practice overemphasize observation and underemphasize the heart of experimental method: intervention. Hoffmann and Pierre Laszlo use the metaphor of Proteus, the Greek sea god who would only foretell the future for those who can seize him to illustrate this point. Proteus avoids detection by changing his form, but Menelaos wrestles with Proteus, pins him down, and makes him talk. Francis Bacon uses the same image, wrestling, to describe the interaction between the scientist and nature. Like Proteus, chemists are also the masters of change, by engineering transformations of molecules. They don't just observe matter, but pin it down, forcing it to speak.

Writing and Communicating Science

As a scientist, Hoffmann understands the role of writing in the creation of scientific knowledge; as a poet, playwright and essayist, he has a deep appreciation of language. Because of his dual perspectives as a scientist and a humanist, Hoffmann has unique insights on scientific communication, particularly the language of chemistry.

The language of chemistry is especially visual. As noted above, a central tenet of chemistry is that the three-dimensional structure of molecules determines properties and reactivity. Chemists have thus developed a language of drawings to represent these structures on the page, what Hoffmann calls chemistry's "iconic vernacular." Typically, substantial portions of chemical articles are occupied by drawings, and even the tables of contents of many chemistry journals are given pictorially. Pictures of structures, reaction schemata, and spectra complement narrative to give a full description of chemical phenomena.

In "Representation in Chemistry," Hoffmann and Pierre Laszlo discuss the intricacies of chemical representation using molecular formulas. Like the characters of any other language, molecular formulas are ultimately symbols, and hence what they denote is intrinsically arbitrary. Their relations of denotation to the structures that they denote are set up according to the conventions of the chemical community. However, the symbols used to denote molecules were not chosen arbitrarily. They were specifically intended to call up a mental picture of the actual structure. At the same time, real molecules are far more complicated than any of their repre-

sentations. Thus, chemists' structural formulas also have a theoretical role. They are abstractions, designed to emphasize those aspects of the molecule that are important for the argument being developed. Therefore, drawing chemical symbols can be viewed both as a rhetorical device and as a form of art, a symbol used by the chemist to communicate with an audience.

Despite being rich with illustrations, chemical articles are often written impersonally and in the third person. But since scientific articles, as opposed to the phenomena they describe, are human constructions, this style of writing is optional. Have scientific articles always been written this way, and is this a good thing? Hoffmann answers both questions negatively. He argues that while early scientific articles were much more discursive and personal, nineteenth-century German chemists struggled to distinguish their work from the more romantic perspective of the *Naturphilosophen.* In the process, they developed a third person, passive style in which facts were emphasized and the role of the investigator suppressed. This has since become the canonical form of the chemical article.

Although this communication system has worked well for nearly two hundred years, Hoffmann argues that the canonical form of the chemical article ought to be changed. He argues that writing in a dry, passive style removes the human side of science. Scientific discovery is a human activity, motivated by epistemic, practical, and even aesthetic considerations. Although scientific knowledge itself must not depend on the discoverer, suppressing the human side misrepresents the actual process of science. Hoffmann argues that when scientific discovery is presented in a more relaxed, autobiographical, and historical format, chemists can more easily "tell their stories." They can emphasize what is most important and communicate the wonder of scientific discovery.

As evidenced by his own prolific career of popular essay writing, Hoffmann also believes that chemists have an obligation to educate the general public. He urges chemists to communicate with the general public so that the citizenry can better understand the chemical issues at stake in public policy. But he also notes that communication with a wider audience requires especially creative thinking about chemistry. This can sometimes lead to new insights and new ideas for research.

Art and Science

Hoffmann is passionate about the fine and performing arts, and that passion pervades his work. He has said that at the end of his college years, he considered making a career of the history of art instead of chemistry, but ultimately lacked the courage to do so. With time, he has managed to find ways to meld his interest in art with his research in chemistry. In 1993, he collaborated with the visual artist, Vivian Torrence, on the book *Chemistry Imagined*, which integrated prose, poetry, and art to communicate chemistry to the general reader. The book was modeled after emblem books of the Renaissance period. His 1995 book, *The Same and Not*

the Same, is similarly a mixture of visual art and chemistry. The three essays in this section explore the connections between art and science, focusing, of course, on chemistry.

Chemists are visualizers; they must be able to imagine and represent the three-dimensional structure of molecules that cannot be seen. Although their thinking about structures is often aided with molecular model kits and, more recently, computer programs, pencil and paper are still the primary tools of the working chemist. One of the skills that an undergraduate must learn is how to draw molecules in ways that show the spatial arrangement of the atoms.

Are these drawings a form of art? Hoffmann argues that they are—not great art, but art nonetheless. Drawings, he tells us, make the molecules come to life. The way that a molecule is drawn emphasizes those aspects of the molecule that the person making the drawing thinks are most important. Sometimes molecular drawings can even be beautiful.

As a science, chemistry owes as much to craft as to natural philosophy. Chemical crafts, such as metallurgy, ceramics, and pharmacy, have a long history, and the skills and techniques of these practical pursuits have found their way into the research laboratory. The synthetic chemist is as much a craftsman as any jeweler; getting a reaction to work can be as delicate a task as throwing and glazing a pot.

In the essay, "Science and Crafts," Hoffmann explores the connections between these two pursuits based on his experiences at the Penland School of Crafts in North Carolina. Most crafts involve some kind of chemistry, usually learned through apprenticeship and practice. Hoffmann asks, "How much chemistry does the craftsman need to know?" Usually, the answer is not much, but a deeper knowledge can be enriching and useful, particularly if the process fails. In that case, a knowledge of chemistry might help in finding and correcting the problem. In chemistry as in craft, hands and minds work together creatively to produce useful, and often beautiful, things.

This leads us to the final question taken up in this section: What, if anything, makes a molecule beautiful? As Hoffmann points out, it is rare to see an aesthetic judgment in a scientific article, but in more unguarded rhetorical circumstances, chemists may remark on the beauty of a particular molecule, just as a physicist or mathematician might say that an equation is beautiful. In "Molecular Beauty," Hoffmann undertakes an investigation of molecular aesthetics.

In some simple cases, molecules are beautiful to the untrained, usually because of their simple but surprising symmetric shapes. Perhaps the most famous molecule of this kind is buckminsterfullerene, the molecular soccer ball. More frequently, substantial chemical background is needed to appreciate chemical beauty. Some of this beauty comes from structure alone, such as the interplay of octahedra in a complicated inorganic crystal or a pair of interlocking rings. In other cases, the beauty comes from function. And in still other cases, the beauty is conceptual, and can be exquisitely concentrated, as when a molecule is created with a single, double, and triple bond all coordinated to the same metal atom.

In considering the criteria for beauty that can be abstracted from these examples, Hoffmann argues that many of these criteria have a counterpoint in classical thinking about esthetics. One major exception he points to involves utility: In most arts, being useful is considered an entirely separate issue from being beautiful. But in chemistry, beauty often comes from molecules and reactions that are especially useful for making other molecules.

Education

Throughout his career, Hoffmann has emphasized the importance of teaching and has been recognized as an outstanding educator, most notably with the George C. Pimentel Award for Chemical Education of the American Chemical Society in 1996. In the late 1980s he took an active part as the presenter and script writer for an influential Annenberg-PBS series of 26 half-hour videos, "The World of Chemistry."

As might be expected, Hoffmann has an unorthodox perspective on teaching and learning that provides the chemical educator with important insights. It is commonplace to say that research improves teaching, but Hoffmann turns that statement around and argues that teaching improves research. In fact, he goes further, by saying that teaching and research are inseparable and symbiotic. However, simply being a good researcher does not automatically make one a good teacher. There are important lessons to be learned both from those who study the teaching and learning process and from successful teachers.

Hoffmann argues that we should view learning not in terms of its location (lecture room, laboratory, etc.) but rather in terms of its audience (undergraduates, graduate students, etc.), noting that audiences often overlap and complement each other. Seen this way, the process of research, which involves developing arguments to convince first oneself and then an expanding series of audiences that something new has been discovered, is essentially the same as teaching. Both involve explaining in words, diagrams, models, and metaphors. Both require clarity of thought and of expression. Both require an understanding of the audience, including what can be assumed and what must be explained.

Those of us who teach undergraduates quickly learn that our students' expectations of the course are different from ours. Hoffmann and Brian Coppola provide us with a nice list of what they call "heretical thoughts on what our students are telling us." Some of the things we consider important, such as providing a broader context, many students find distracting. As we push them to understand principles and see the big picture, students find that memorization and compartmentalization are often effective learning strategies. These lessons from students are important, but as professionals and expert learners, we need to design courses that communicate what is essential and valuable about chemistry.

Along with their philosophical and theoretical perspectives, teachers also need techniques, practical suggestions on ways to help students learn. Based on forty years of experience, Hoffmann, along with Saundra Y. McGuire, provide the working teacher with some down-to-earth advice supported by references to the teaching and learning literature showing why these techniques actually work. Some of the advice seems obvious: Students should take lecture notes by hand, then rework them after class. But there are good reasons, based on cognitive research, why this old idea is still a good idea. The suggested strategies are all ones that promote active learning by taking advantage of a productive interplay of group and individual learning. But technique needs to be supplemented by empathy and empowerment. Teaching is a relational human activity and the human connection is essential.

Ethics in Science

Hoffmann has not written many articles that discuss ethics explicitly, although moral considerations are an important subtext in much of his writing. The four essays in this section, including two previously unpublished lectures, grapple with several important ethical questions involving chemistry, particularly concerns about environmental degradation.

The essence of Hoffmann's ethical stance can be found in the title of his *Chemical and Engineering News* editorial: "Mind the Shade." Humans are constantly presented with ethical decisions, few of which are black and white. Because of the natural tendency to rationalize, compartmentalize, and diffuse responsibility for actions that result in hurt, it is essential that we pay special attention to those moral decisions that are in the gray area. Because chemists create new molecules and new understanding of the natural world, they need to be mindful of the consequences of their discoveries. It is too easy to say that the responsibility lies with those who use our creations, and not with the creator.

Where do we look for guidance in making those difficult decisions in the shade? Hoffmann reminds us of the work of Jacob Bronowski, who pointed out that the practice of science leads to the "habit of truth." Experiment helps to keep us honest as does the reporting of experiment. There are those who believe that science is ethically neutral, but Hoffmann rejects this view. He believes that "the invention or implementation of a tool without consideration of the consequences of its use is deeply incomplete." Much of his ethical writing explores this theme, pointing out that chemists are forced to make moral choices, whether they like it or not.

One of the most important contemporary ethical issues is environmental degradation. The marvelous inventions of modern chemistry have been accompanied by environmental damage that, in Hoffmann's view has moved from just being a mess to what he characterizes as something like a sin. It would be easy to scold the industries

responsible for environmental degradation, but Hoffmann chooses instead to make practical suggestions for how to make chemistry more ethical. Industry will adopt green chemistry practices if they make economic sense; the bigger problem is in the academy where green chemistry is often regarded as uninteresting. Making new compounds is sexy; developing a green process to make an industrially useful compound may seem boring. More federal funding will certainly attract interest, but more important is a change in attitude among academic chemists.

A good model for how green chemistry could thrive in academic departments can be found in the history of polymer chemistry. Once considered second-rate, applied chemistry, polymer chemists are now in high demand in chemistry departments and they seem to have no trouble attracting good graduate students to their research groups. Part of this new found legitimacy is due to the work of some first rate academic chemists, such as Robert Grubbs, who found that polymer synthesis presented some fascinating area of research. Green chemistry needs similar role models. It also needs a different pedagogical approach, one that emphasizes the particular. Case studies can provide an entry point for students, showing them the intellectual puzzles that make chemistry so irresistible.

A final ethical contribution is Hoffmann's suggestion of a new way to evaluate green chemical technologies. He suggests the creation of a "transformation index," a new way of measuring efficiency primarily based on thermodynamic considerations, but that also recognizes ethical dimensions.

In the end, the answers to these broad ethical questions depend on our values which in turn reflect our vision of ourselves as human beings. Here Hoffmann turns to Genesis, which contains two creation stories that show the two sides of the human character: the creative transformer of nature and the keeper of the garden. Both sides of the human personality are needed for complete ethics of science.

Conclusion

Roald Hoffmann's perspective on science derives from his unusual career as a successful theoretical chemist who collaborates closely with experimentalists, and his parallel career as a writer of essays, poems, and plays. Hoffmann's research has ranged broadly through organic, inorganic, and solid state chemistry. His writing outside of science encompasses both scientific and nonscientific themes. In a world where scholarship has become increasingly specialized, Hoffmann's interdisciplinary perspective provides unique insights into the philosophy of science in general and the philosophy of chemistry in particular.

Hoffmann's view is that chemistry, at its core, is a creative human activity in which synthesis, making new molecules, plays a central role. Because of the importance of synthesis to chemistry, chemical explanations must employ those sometimes fuzzy, purely chemical concepts that the experimental chemist can readily use to design

and control chemical reactions. Chemical communication is likewise a creative human activity that involves both words and a unique iconic vernacular of drawings that represent the three-dimensional molecular structures that determine chemical properties. Through both the drawings that decorate the typical chemical article and the historic connections with the craft tradition, chemistry has surprising connections to art. Finally, because chemists create new substances, they incur a moral responsibility to consider the consequences for society of the use of the materials they make. Hoffmann provides us with a truly human and humane philosophy of science.

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1

Trying to Understand, Making Bonds

ROALD HOFFMANN

In 2007, on the occasion of my 70th birthday, Bassam Shakhashiri organized a symposium for me at the Boston meeting of the American Chemical Society. The session was entitled "Roald Hoffmann at 70: A Craftsman of Understanding." I began my talk with thanks to many. That section has been shifted to the end of this chapter.

Beginnings

I was born in a happy young Jewish family in unlucky times, 1937. In that war, most of us perished, 3800 of the 4000 Jews of Złoczów, now Zolochiv in Ukraine. Among those who were killed were my father, three of four grandparents, three aunts, and so on. I just want to show you three photos which relate to that time, one old and two recent. The last 15 months of the war we were hidden by a good Ukrainian man–Mikola Dyuk, the schoolteacher in the small village of Univ. The first year we were in an attic of the schoolhouse, the second year in a storeroom with no windows, maybe 6 x 10 feet, on the ground floor.

Here are two photos from 2006, when my sister, my son, and I visited Univ. Here is the attic in which we were hidden, with its one window (Figure 1-1).

The storeroom, a passageway, another ground floor room are gone, rebuilt into a new classroom of Univ's school.

It's a chemistry classroom (Figure 1-2). Such is fate. Under the plank floor we dug a bunker to sit in if the police came to the house.

I was five and a half when we went in. And nearly seven when we went out. Here's a photo of me, a few months after we came out (Figure 1-3).

We survived. Some of us. Good people helped us, I tell their story. I am also the speaker for the dead—the three million Polish Jews who were killed do not have good stories to tell, or photos to show.

We built a new life, in refugee camps where I read of Marie Curie and George Washington Carver, and then came to America in 1949.

(a)

(b)

Figure 1-1 (a) The attic of the Univ schoolhouse, (b) and the schoolhouse itself, where Roald, his mother, and three others were hidden in 1943.

Then we lived happily ever after! Or, to put it another way—it was wonderful, the only unhappiness in our lives put there by ourselves and no one else. My mother said I must never say anything bad about America.

Moving toward Chemistry

I got to our science sideways, so to speak. By first going toward (under parental pressure) medicine, then edging away. Not having enough courage to go into the humanities—that wonderful opening up of the world to me at Columbia, which you can sense in my mention of my teachers at the end of this chapter. Even in my

Figure 1-2 A present day chemistry classroom, Univ, Ukraine, in the space where Roald and relatives were hidden in 1944.

Figure 1-3 First photograph of Roald after war, in fall 1944, age 7.

first two years in graduate school at Harvard I wasn't sure about chemistry—I sat in on courses in astronomy, public policy, archaeology. Going to the Soviet Union for a year was a way to avoid commitment.

When I came back in 1961, I knew chemistry was my science. I did my Ph.D. work in one productive year.

You know what I've done, with more than a little help from my friends. I want to talk here about some lines that seem to emerge, ever so faintly, from more than 45 years of scientific activity.

The Rhetoric of Pedagogy

So the chairman of the department (Harold Scheraga) said more or less this: "We thought that after teaching physical chemistry lab, you might want to try an introductory chemistry course." Jim Burlitch and I did as we were told, and rebuilt an honors course that had withered. We were lucky; in that course were Cornell's brightest students. And I learned how to explain to them thermodynamics without those partial derivatives.

I've taught introductory chemistry every year since; I finished teaching at Cornell with two such courses. The pedagogical imperative entered my research. I was in the business of explaining anyway—in time I realized that most of the difference between teaching an introductory course and writing my technical papers was in the audience—the strategies of communication were different on the surface, but underneath similar.

As a result of teaching, my research improved. I wanted people to understand—students, researchers. So I tried, using colloquial language, using strategies of optimal redundancy, many pictures, an occasional poke of colorful language to wake people up. No mysteries (beyond those of nature) were to be created. And if one could communicate to the reader (so much easier in a lecture) that I cared that they understand, I was home free. They learned.

I've always written my papers not for my colleagues, but for the 3rd year graduate student.

Calculations and Explanations

My research career is intimately tied to the computer age; there are all those tables in my very first theoretical chemistry paper, with Lipscomb. An IBM 604 diagonalized that matrix for $C_2B_{10}H_{12}$. The sound of the key punch is deeply embedded in my consciousness. As is FORTRAN. But from the beginning, there was this love-hate relationship I had with calculations. For Lipscomb emphasized symmetry and structure, and the work with Woodward taught me the tremendous power of a qualitative argument.

I could sense that the qualitative arguments, based on perturbation theory, were appreciated, used, and cited by people. I think I understood this firmly for the first time (outside of the context of the work I did with RBW) in my initial independent studies at Cornell—on the way a methylene approaches an ethylene, and in the explanation (through bond coupling) of the large splitting of the lone pair orbitals of pyrazine or diazabicyclooctane.

The tension is exacerbated in our times, as simulation crowds out model-building. I've written of this elsewhere.[1]

I was lucky; I became an explainer in an age that needed them. Now how much of explaining is telling just-so stories, you will have to decide. The stories I've told—of orbitals, of two and four electron two-orbital interactions, of through-bond coupling, the isolobal analogy, of a fragment MO analysis, of crystal orbital overlap populations, of how bands run, and bonds and bands in general—are pretty good ones; they have a way of holding on.

I'm very proud of teaching chemists (together with Jeremy Burdett and Mike Whangbo) the connection between the language and phenomena of solid state physics, of extended periodic systems and the molecular orbital theory of discrete molecules. As for motion in the other direction, convincing physicists that there is value in chemical intuition on bonding, well, the best I can say is that I haven't given up trying…

The Graphical Imagination, or Why Orbitals Matter

So organic and inorganic chemists, with no artistic training, became in the 20th century masters of simple 3-dimensional communication. The context was molecular structure; I am thinking of drawing a chair cyclohexane, benzene-$Cr(CO)_3$, or the organometallic molecules shown in Figure 1-4.

All along, people were drawing orbitals and using them. Leslie Orgel's work in inorganic chemistry in the sixties in exemplary, as is Howard Zimmerman's stereoelectronic reasoning in the organic realm. So there was nothing novel in what we did (now that is a recurring theme, and true), only a persistent, pedagogically informed application of orbitals and interaction diagrams to one real chemical case after another, to a multitude of bonding puzzles, to build frameworks of understanding of some generality, in a language accessible to that 3rd year graduate student.

The net result of hundreds of interaction diagrams of the kind you see here (Figure 1-5) is the grafting of electronic information in a graphical code onto an already existing stereochemical imagination. So, just as molecules could be seen as structures made up of a framework of definite three-dimensionality, with functionality (donors, acceptors, chromophores) geometrically dispersed on that framework, the same molecules could be furnished, so to speak, with orbitals, and those would explain and control reactivity, color, etc.

The necessary orbital theory was within reach of an intelligent graduate student; driven by my teaching instincts (and maybe my deflected art historical interests) we created a pictorial perturbation theory that seemed to be psychologically just right for the sophistication of the community. Michael Dewar couldn't understand how people didn't take to his numerical perturbation theory for organic chemistry—after all, it had everything in it. It did. But it was not taught nor used, just because it was not graphic. People like pictures. Chemists live off them.

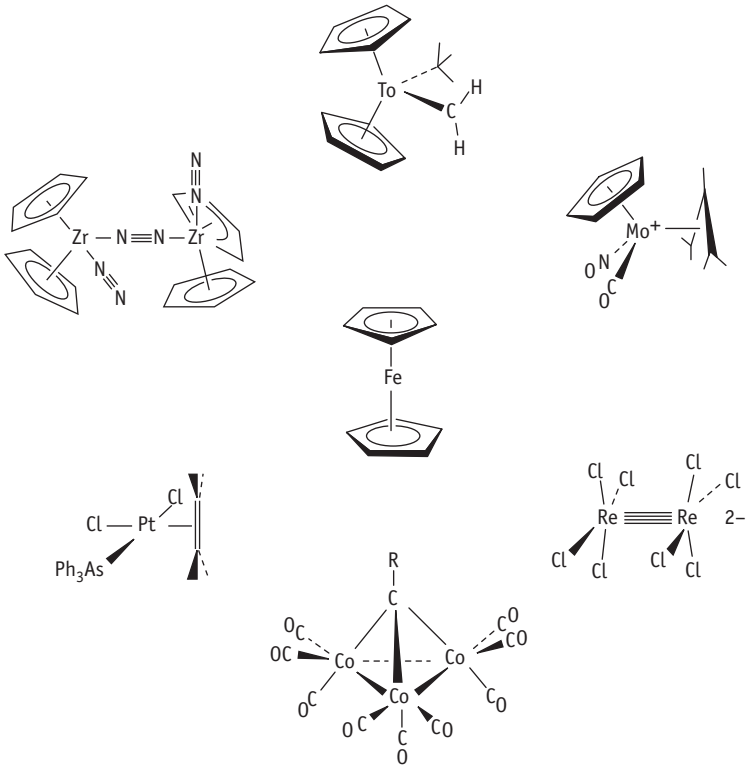

Figure 1-4 Some typical organometallic compounds.

Building Bridges, Making Bonds

I believe leitmotifs emerge, they are not programmed. If someone asked me, "Roald Hilelovich, what is your philosophy of research?" I'd answer—as I answer all your mail, some by hand because my mother, the strong force in my life, said you have to answer mail—I'd answer, "I don't work on important problems, I work on what the world gives me. I am an amoeba." Now this is said in part for effect, I am, after all, a writer. But here is what I mean—the world is complex and particular, the bead of dew on that blade of grass, and no other blade, no other dew, no other observer than me. And the world is connected—the drop's water is my water, the grass blade's biochemistry has much overlap with mine, the chlorophyll is green whether in that blade or in R. B. Woodward's synthesis. There are differences—the weed respires in a way different from me. The differences are telling.

I have patience. And like a figurative omnivorous amoeba I will look at, listen to, taste anything in this world—organic or inorganic, heavy metal or Bach, Korea or Brazil. I will transform the riches of the world not as an amoeba, but as a human

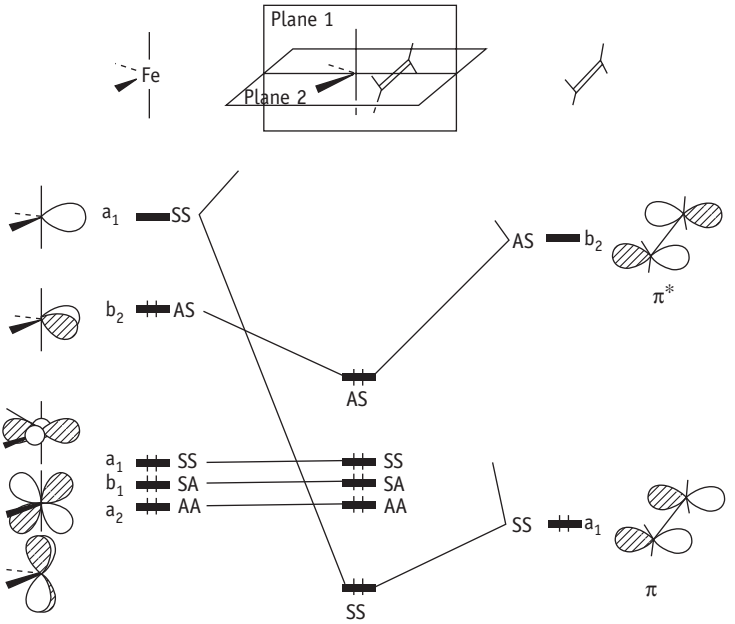

Figure 1-5 An orbital interaction diagram for $(CO)_4Fe$(ethylene). Note the mix of stereochemical drawings and orbitals.

being. Which means I will try to understand the disparate chemical aspects of a rich universe (and not just the chemistry), try to see relationships between them. My faith—not a religious one, but certainly a spiritual one—is that the connections are there, that our humanity lies in seeking such connections.

I've been lucky, within theoretical chemistry. A method came my way—extended Hückel theory, but more broadly qualitative molecular orbitals and the perturbation theory-based way of following their interactions. That method could be used on any molecule under the sun. The fragment molecular orbital analysis attached to this methodology took molecules apart, and put the pieces together, on paper. This permitted connections to be made—one could see similarities, while at the same time the differences emerged in a way consilient with chemical thinking, with variations in electronegativity and donor and acceptor character.

I used that gift which came my way to make connections. So my Nobel Lecture is not a looking back to the story I am immensely proud of, the complex of orbital symmetry ideas developed with R. B. Woodward. Instead, the lecture sets out the isolobal analogy, under the title of "Building Bridges between Inorganic and Organic Chemistry."

In time I came back to my love for the word and for art, and slowly began to build connections between chemistry and the makers of the spirit—artists, writers, actors, performers, religious thinkers. I could do this only by entering their world,

on their terms—the world of struggling to get a poem published, or a play produced. I did this; it remains hard, but tremendously satisfying.

Quiet Subversion, and Fun

By this I mean many things, inter alia my gentle campaign to relax the constraints of the ossified format of a scientific article, or of journals for that matter. I am very proud of having convinced the nonpareil editor of *Angewandte Chemie*, Peter Gölitz, to publish essays. The *Journal of the American Chemical Society* and *Physical Review* wouldn't dream of doing it, right? In an article on silver fluorides, we were allowed to insert a commentary by a sage protagonist, Neil Bartlett, into the text. We could write a discussion on valence bond and MO theory as a dramatic trialogue.

Fun: I think science is fun, as does Bassam, even as it is as serious as a search after reliable knowledge, knowledge that can hurt or heal, must be. The gatekeepers won't let you crack jokes in a paper, but one can be playful in the heart of science. A recent paper on squeezing CC bonds we did traipsed through a jungle gym of organic structures in the service of torturing a nice normal CC bond. The work Roger Alder, Charlie Wilcox, and I once did on square planar carbon was I think, in its own way, compassionate. What could be done, electronically, to give comfort to this unhappy structure?

In the "Entertaining Science" cabaret I run monthly in New York City, we juxtapose science with performance—music, dance, theater, magic. The audience makes every connection we want, and then some. They laugh, with affection, at everything we do. Even I, an awfully serious character (not really), can come off as Harry Gray.

Emotional Engagement

You can't write poetry without it, nor without personal exposure. But I'm speaking of other things as well. It seems to be given to me to be faced with ethical problems. I did not evade the painful consideration of E. J. Corey's claim of having told R. B. Woodward of the MO argument for control of electrocyclic reactions. Nor have I avoided thinking about the actions of Peter Debye in prewar Germany. And in returning to Złoczów, the place where I was born, in 2006, we, the survivors and their children, were drawn into the agony of remembering, and forgiving. There are times I wish I had been spared; but then I reflect, and I am thankful to the world for giving me the opportunity to face them.

I think I've been a good teacher because I've allowed the emotional into what passes between me and my students. So I've been able to communicate to students that the subject is ever new to me, and that I care that they learn, and I care about them as human beings.

We have come full circle. There is a time to thank: For the existential act of living, day by day; the wonder of connections out there to be seen; the microcosm of chemistry; the power of art and the word; the great reach of explaining and teaching with feeling. For being able to try to do these things, ultimately to teach and to retain the desire to be taught, for this I am grateful.

So, at 70, let me give thanks:

1. To the people who saved us in the war: Mikola Dyuk and his wife Maria.
2. To the people who ran the education program in the U. S. Occupation Zone in postwar Germany; aside from doing it well, they sponsored the translation of books, so-called Overseas Editions, meant to set Germans on a democratic path. Two of these inspired a 10-year-old boy in a refugee camp in Wasseralfingen: Eve Curie's hagiography of her mother, and Rackham Holt's life of George Washington Carver. I read these in German.
3. To my teachers at P. S. 93, Queens (especially my cousin, Sally Stewart), at P. S. 16, Brooklyn, Nathan Green and Abe Schwartz, and at Stuyvesant H. S., especially Abe Penzer, a great biology teacher.
4. To Abraham Wajngurt, a landsman who worked in the stockroom at Yeshiva University, and here and there slipped me pieces of chemical glassware.
5. To a great teaching assistant at Columbia, Bob Schneider. And two chemistry teachers there who introduced me to quantum mechanics: George Fraenkel and Ralph Halford.
6. To the teachers at Columbia, who opened up the world to me: Mark Van Doren, Donald Keene, Howard McParlin Davis, and Martin Ostwald.
7. To the people who introduced me to research, in summer jobs at the National Bureau of Standards: Ed Newman, Bob Ferguson, and at Brookhaven National Laboratory: Jim Cumming.
8. To my Ph.D. Advisors: Martin Gouterman and William Lipscomb. For both I was their first graduate student at Harvard.
9. To Per-Olov Löwdin and his Summer School in Sweden, where I learned group theory and met my wife.
10. To the IREX exchange, which brought me to Moscow for a year in the middle of graduate school, against Harvard's and my family's wishes.
11. To the Society of Fellows, for three years of freedom which allowed me to learn organic chemistry. During that time, it was E. J. Corey who, by simply telling me of his work, got me deeply interested in organic chemistry.
12. To R. B. Woodward, intellect incarnate, the patterner of chaos. He allowed a pair of helping hands to be transformed into a collaborator, and, over the years we worked together, ever so subtly pushed me from calculation to explanation.
13. To Cornell, for having faith and offering me a job, when I had sullied a good theoretical reputation by doing organic theory.

14. To Chem. 215, and 216, and 207, and 208, and 103, and 106, and 206 all the introductory chemistry courses I taught.
15. To my Cornell colleagues, for collegiality over four decades.
16. To Cornell again, to two Presidents: Dale Corson and Frank Rhodes, who supported me in so many ways.
17. To places that gave me intellectual shelter on sabbaticals and leaves: the ETH Zurich, the Universities of Stockholm and Lund in Sweden, Cambridge University, Moscow State University, NYU, and Columbia.
18. To my secretaries and assistants over the years, Valerie Watt, Eda Kronman, Joyce Boda, Ellie Stagg, Patricia Giordano, Jenny Cleland, and Catherine Kempf.
19. To Jane Jorgensen, the mistress of the lined orbital, who did my drawings over the years.
20. To my graduate students over 42 years: Chien-Chuen Wan, David Hayes, Jerrald Swenson, James Howell, Maynard M. L. Chen, David L. Thorn, Birgitte E.R. Schilling, Charles N. Wilker, Steve Cain, David M. Hoffman, Kevin Haraki, Timothy R. Hughbanks, Sunil D. Wijeyesekera, Shen-shu Sung, Chong Zheng, Ralph A. Wheeler, Marja C. Zonnevylle, Yat-Ting Wong, Edith A. Chan, Jing Li, Zafiria Nomikou, Kimberly Lawler-Sagarin, Michael Bucknum, Qiang Liu, Hugh Genin, Grigori Vajenine, Gregory Landrum, Abds-Sami Malik, Erika Merschrod, Garegin Papoian, Wingfield Glassey, Ying Wang, Melania Oana, Mihaela Bojin, Daniel Frederickson, Pradeep Gutta, Chinmoy Ranjan, Nicholas Gerovac, Ji Feng, and Anne Poduska.
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Ruedi Rytz, Robert Konecny, Ralf Stowasser, Jesus Ugalde, Dong-Kyun Seo, Nguyen Trong Anh, D. M. P. Mingos, Jeremy Burdett, Paul Dobosh, John Eisch, Clifford McGinn, Victor Tortorelli, Evgeny Shustorovich, Robert Bach, Richard Harcourt, San-Yan Chu, Helga Dunken, Yuansheng Jiang, Debbie Fu-tai Tuan, Daniel Zeroka, Reinhard Nesper, Jingling Huang, Maria José Calhorda, P. A. Cox, John Lowe, Mikhail Basilevsky, Peter Kazmaier, Vladimir Minkin, Gion Calzaferri, Boris Simkin, Maria Matos, Hassan Rabaâ, Donald H. Galván, Sung Hong, Jürgen Evers, Valeria I. Rozenberg, Hoseop Yun, Lan-Feng Yuan, Antonio B. Hernandez, Ray Torralba, Kee Hag Lee, Wojciech Grochala, Andrea Ienco, Pattath Pancharatna, M. M. Balakrishnarajan, Beate Flemmig, Carol Parish, Deborah Huntley, Gabriel Merino, Dean Tantillo, Peter Kroll, Marketa Munzarova, Kelling Donald, Jason D'Acchioli, Edyta Greer, Warren Hehre, Roy R. Gould, Peter Rossky, Karen Goldberg, Robert Weber, Geoffrey Zeiss, Chris Zeiss, Leigh Ann Henderson, Mikhail Velikanov, Lori Rayburn, Stephen Goldberg, Jeffrey R. Long, Aliya Courtney, Pooja Pathak, Georgios Markopoulos, Tomasz Jarón, Tom Cahill, Milan Randić, Ming-Der Su, Sergei Kryutchkov, Mikhalil Grigoryev.

Special thanks to the German, French, and Japanese science research agencies – DAAD, DFG, CNRS, JSPS – which kept a steady flow of postdocs coming from these countries.

22. The National Science Foundation has supported my work for 50 years. Except for a lapse several years ago, they have provided most of the economic base for my free-ranging research. I hope I've repaid their confidence in my science.
23. My literary collaborators – the editors at *American Scientist*; coauthors R. B. Woodward, Vivian Torrence, Shira Leibowitz Schmidt, and Carl Djerassi.
24. And my family; not a large one, but consistently supportive of what I have done over the years: my mother Clara, who died in 2006, who led our family group in the period of survival, my father Hilel Safran (1911–1943), my stepfather Paul Hoffmann (1904–1981), my sister Elinor, my wife Eva, and my children Hillel Jan and Ingrid Helena. Who, between them, took exactly one semester of chemistry.

Note

1. R. Hoffmann, Qualitative Thinking in the Age of Modern Computational Chemistry, or What Lionel Salem Knows. *J. Mol. Str. (Theochem.)* 424 (1998): 1. Chapter 7 in this book.

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Part 1

CHEMICAL REASONING AND EXPLANATION

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2

Why Buy That Theory?

ROALD HOFFMANN

The theory of theories goes like this: A theory will be accepted by a scientific community if it explains better (or more of) what is known, fits at its fringes with what is known in other parts of our universe, and makes verifiable, preferably risky, predictions.

Sometimes it does go like that. So the theory that made my name (and added to the already recognized greatness of the man with whom I collaborated, *the* synthetic chemist of the 20th century, R. B. Woodward) did make sense of many disparate and puzzling observations in organic chemistry. And "orbital symmetry control," as our complex of ideas came to be called, made some risky predictions. I remember well the day that Jerry Berson sent us his remarkable experimental results on the stereochemistry of the so-called 1,3-sigmatropic shift. It should proceed in a certain way, he reasoned from our theory—a non-intuitive way. And it did.

But much that goes into the acceptance of theories has little to do with rationalization and prediction. Instead, I will claim, what matters is a heady mix of factors in which psychological attitudes figure prominently.

Simplicity

A simple equation describing a physical phenomenon (better still, many), the molecule shaped like a Platonic solid with regular geometry, the simple mechanism (A→B, in one step)—these have tremendous *aesthetic* appeal, a direct beeline into our soul. They are beautifully simple, and simply beautiful. Theories of this type are awesome in the original sense of the word—who would deny this of the theory of evolution, the Dirac equation or general relativity?

A little caution might be suggested from pondering the fact that political ads patently cater to our psychobiological predilection for simplicity. Is the world simple? Or do we just want it to be such? In the dreams of some, the beauty and simplicity of equations becomes a criterion for their truth. Simple theories seem to

validate that idol of science, Ockham's Razor.[1] In preaching the poetic conciseness and generality of orbital explanations, I have succumbed to this, too.

A corrective to the infatuation of scientists with simplicity might come from asking them to think of what they consider beautiful in art, be it music or the visual arts. Is it Bach's Goldberg Variations or a dance tune where the theme plays ten times identically in succession? Is any animal ever *painted* to emphasize its bilateral symmetry?

Still, there's no getting away from it; a theory that is simple, yet explains a lot, is usually accepted in a flash.

Storytelling

What if the world is complex? Here, symmetry is broken; there, the seemingly simplest of chemical reactions, hydrogen burning to water, has a messy mechanism. The means by which one subunit of hemoglobin communicates its oxygenation to a second subunit, an essential task, resembles a Rube Goldberg cartoon. Not to speak of the intricacies of *any* biological response, from the rise of blood pressure or release of adrenalin when a snake lunges at us, to returning a ping-pong serve with backspin. Max Perutz's theory of the cooperativity of oxygen uptake, the way the ribosome functions—these require complicated explanations. And yes, the inherent tinkering of evolution has made them complex. But simpler chemical reactions—a candle burning—are also intricate. As complex as the essential physics of the malleability, brittleness and hardness of metals. Or the geology of hydrothermal vents.

When things are complex yet understandable, human beings weave stories. We do so for several reasons: A→B requires no story. But A→B→C→D, and not A→B→C'→D *is* in itself a story. Second, as Jerome Brunner writes, "For there to be a story, something unforeseen must happen." In science the unforeseen lurks around the next experimental corner. Stories then "domesticate unexpectedness," to use Brunner's phrase.[2]

Storytelling seems to be ingrained in our psyche. I would claim that with our gift of spoken and written language, this is the way we wrest pleasure, psychologically, from a messy world. Scientists are no exception. Part of the story they tell is how they got there—the x-ray films measured over a decade, the blind alleys and false leads of a chemical synthesis. It is never easy, and serendipity substitutes for what in earlier ages would have been called the grace of God. In the end, we overcome. This appeals, and none of it takes away from the ingenuity of the creative act.

In thinking about theories, storytelling has some distinct features. There is always a beginning to a theory—modeling assumptions, perhaps unexpected observations to account for. Then, in a mathematically oriented theory, a kind of development section follows. Something is tried; it leads nowhere, or leaves one dissatisfied. So one essays a variation on what had been a minor theme, and—all of a sudden—it soars. Resolution and coda follow. I think of the surprise that comes from doing a

Fourier transform, or of seeing eigenvalues popping out of nothing but an equation and boundary conditions.

Sadly, in the published accounts of theories, much of the narrative of the struggle for understanding is left out, because of self-censorship and the desire to show us as more rational than we were. That's okay; fortunately one can still see the development sections of a theoretical symphony as one examines an ensemble of theories, created by many people, not just one, groping toward understanding.

The other place where narrative is rife is in the hypothesis-forming stage of doing science. This is where the "reach of imagination" of science, as Jacob Bronowski referred to it, is explicit. Soon you will be brought down to earth by experiment, but here the wild man in you can soar, think up any crazy scheme. And, in the way science works, if you are too blinded by your prejudices to see the faults in your theoretical fantasies, you can be sure others will.

Many theories are popular because they tell a rollicking good story, one that is sage in capturing the way the world works and could be stored away to deal with the next trouble. Stories can be funny; can there be humorous theories?

A Roll-On Suitcase

Theories that seek acceptance had better be *portable*. Oh, people will accept an initiation ritual, a tough-to-follow manual to mastering a theory. But if every application of the theory requires consultation with its originator (that's the goal of commercialization, antithetical to the ethic of science), the theory will soon be abandoned. The most popular theories in fact are those that can be applied by *others* to obtain surprising results. The originator of the theory might have given an eyetooth to have done it earlier, but friends should hold him back—it's better if someone else does it. And cites you.

Relatively uncomplicated models that admit of an analytical solution play a special role in the acceptance and popularity of theories among other theorists. I think of the harmonic oscillator, of the Heisenberg and Hückel Hamiltonians, of the Ising Model, my own orbital interactions. The models become modules in a theoretical *Aufbau,* shuttled into any problem as a first (not last) recourse. In part this is fashion, in part testimony to our predilection for simplicity. But, more significantly, the use of soluble models conveys confidence in the value of metaphor—taking one piece of experience over to another. It's also evidence of an existential desire to try something—let's try this.

Productivity

The best theories are productive, in that they stimulate experiment. Science is a wonderfully interactive way for gaining reliable knowledge. What excitement