Roald Hoffmann: An Appreciation Jay A. Labinger Beckman Institute California Institute of Technology

Abstract

Roald Hoffmann's unsurpassed accomplishments on both sides of the humanities/sciences border (which much of his career has been aimed at demolishing) have been recognized, *inter alia*, by the 2022 SLSA Lifetime Achievement Award and the 1981 Nobel Prize in chemistry. His work spans a wide range of SLSA-related topics — the creative nature of science in general and chemistry in particular, the central role of narrative in scientific investigation and reporting, the nature of the scientific article, the importance of artistic representation for chemistry, and others — in addition to producing several science-themed plays and an extensive body of poetry, as well as making chemistry accessible to the non-specialist. This essay highlights some of his most significant contributions to SLSA's mission and goals.

Paper

Roald Hoffmann is the recipient of the 2022 SLSA Lifetime Achievement Award. He is only the second practicing scientist to receive it (the other was physicist Sidney Perkowitz, in 2015) — perhaps not surprisingly, given the relative paucity of active scientists in SLSA, or literature and science (henceforth L&S) more generally¹ — and surely the most recognized for his scientific work, with many honors including the 1981 Nobel Prize in chemistry. His nontechnical work, which has manifested itself in essays, plays, poetry, and other forms, eloquently demonstrates how the similarities between the activities in which scientists and humanists are engaged vastly outweigh any differences. Here I highlight a selection of his writings that display both the breadth and depth of his contributions, as well as some of the flavor of his style(s).

Roald's scientific career has been primarily in the field of theoretical/computational chemistry, in which he has published over 650 articles to date. I will not go into that in any detail for this essay, but I do want to note that he has always striven to present his results so that they may be made readily accessible and useful to non-experts — what he calls "applied theory" — by emphasizing pictorial displays and qualitative explanations over simple numerical readouts. (That is not to say that his calculational work is anything other than rigorous!) A prime example is his work on the so-called Woodward-Hoffmann rules, for which his Nobel Prize was awarded. The rules are used to predict stereochemical outcomes of a variety of organic reactions on the basis of symmetry alone; the concise but compelling book describing them² contains not a single calculated number. It seems clear to me that these scientific inclinations and his non-technical, humanistic interests arise from the same impulse.

He has been nearly as prolific on the non-technical side, with over 200 articles (besides the afore-mentioned poetic and dramatic work), many of which have been collected in four major books. Two of those, both explicitly aimed at making chemistry interesting for non-

¹ Jay A. Labinger, "Where Are the Scientists in Literature and Science?" *Journal of Literature and Science* 10. no. 1 (2017): 65-69.

² R. B. Woodward and R. Hoffmann, *The Conservation of Orbital Symmetry* (Weinham: Verlag Chemie, 1971).

chemists, employ somewhat different unifying principles (although there is considerable thematic overlap). The first published, *Chemistry Imagined*,³ is the outcome of a collaboration with artist Vivian Torrence. Consisting of some 30 short essays and poems, each accompanied by a collage-like illustration, it was the basis of exhibitions at a number of academic and scientific institutions, as well as for the plenary talk Roald gave at the 1996 meeting of SLS (then not yet SLSA) in Atlanta. The subtitle for that presentation was "Delight and Tension in an Art/Literature/Science Collaboration;" the abstract promised (and Roald delivered, to my recollection) "observations on…where the context of juxtaposition leads, and how text and image, mystery and clarity, fared in this collage of a collaboration."

Rather than looking more deeply into that work, I will focus on the second, which appeared shortly afterwards: *The Same and Not the Same.*⁴ As noted, some of the individual essays in this collection address topics which are also considered in *Chemistry Imagined*; but here the main idea is juxtaposition — not of science and art, but of paired, often opposing, dualities, also expressed by the Atlanta plenary's reference to "delight and tension...mystery and clarity." As Roald suggests in his Preface, the conceit inherent in the title, which is put forth as central to chemistry, is applicable elsewhere:

The dualities — of molecules and the process of their making — are important, I think, in forming a link between the chemist and the non-chemist. It is possible to answer the question "What do I have?" and to reflect on whether the substance made is the same or not the same as others. But why is that question interesting? Because the question of identity, of *our* identity, shaped in childhood in a complex dance of bonding and separation, matters deeply to us. The processes of nature connect with the interior world of our emotions.⁵

I would argue that this idea is particularly relevant to L&S, given the importance that so many of its practitioners have ascribed to the role of *metaphor* in connecting the domains.⁶ What is a metaphor, after all, but a means of showing how two things (ideas, concepts) are at once the same and not the same? There is no explicit statement of this connection in *The Same and Not the Same*, but I think it very likely that it was somewhere near the forefront of Roald's mind as he put the book together: a number of the *many* references to metaphor that appear throughout link chemistry to literature and other extra-scientific realms. In his very first chapter, "Lives of the Twins," he starts with an excerpt from a Joyce Carol Oates book of the same title⁷ to preview the entire book — with emphasis on the work done by metaphor:

In this book the essential tensions of chemistry will be explored; I will seek the polarities that power, rend, and reform the world of molecules. What *do* twins have to do with it? Everything. The questions implicit in Molly Marks's description of the twins are "Who are you?"; "Are you different?"; "Are you the

³ Roald Hoffmann and Vivian Torrence, *Chemistry Imagined: Reflections on Science* (Washington: Smithsonian Institution Press, 1993).

⁴ Roald Hoffmann, *The Same and Not the Same* (New York: Columbia University Press, 1995).

⁵ Ibid., *xv-xvi*.

⁶ Jay A. Labinger, *Connecting Literature and Science* (New York: Routledge, 2022), 51-59.

⁷ Rosamond Smith, *Lives of the Twins* (New York: Simon & Schuster, 1987).

same?" The tension for Molly is that of recognition, of identity, of the same and not the same. The same overpowering questions initiate the dialogue of a chemist with recalcitrant matter. He or she also asks, "What are you?"; "Are you different?"; "Are you the same?" The stranger within; the idea of molecular mimicry — these guiding metaphors of immunology and drug design extend the notion of molecular identity. They are strong metaphors, as we shall see, because they touch deep concerns of differentiation, of individuation, of the self.⁸

One of Roald's main duality themes is that of discovery vs. creation:

In describing what they do, scientists have by and large bought the metaphor of discovery, and artists that of creation. The cliché "uncovering the secrets of nature" has set, like good cement, in our minds. But I think that the metaphor of discovery is effective in describing only part of the activity of scientists, a smaller piece still of the work of chemists....What is strange is that chemists should accept the metaphor of discovery. Chemistry is the science of molecules....Some if the molecules are indeed *there*, just waiting to be known by us....But so many more molecules are made by us, in the laboratory....The situation is not all that different from the artist who, constrained by the physics of pigment and canvas, and shaped by his or her training, nevertheless creates the new.⁹

I don't suppose Roald wants to suggest that chemists should feel a sense of superiority — in that their field is even *more* closely connected to the arts and humanities than science in general — but maybe a *little* of that is not totally unjustified? In his "Personal View of Chemistry," from an article republished in the most wide-ranging collection of his essays,¹⁰ he comments:

I take discovery in the sense of revealing some perhaps obscured laws of nature, creation in the sense of making new things. In describing their work most scientists will stress the discovery metaphor, while most artists will emphasize creation. Well, I think much of what we do in science is creation. Especially so in chemistry.¹¹

A key principle of Roald's understanding of how knowledge is both generated and disseminated is that of *narrative*. He observes:

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....Sadly, in the published accounts of theories, much of the narrative of the struggle for understanding is left out....The

⁸ Hoffmann, *The Same and Not the Same* (above, n. 4), 6.

⁹ Ibid., 87-90.

¹⁰ Jeffrey Kovac and Michael Weisberg (eds.), *Roald Hoffmann on the Philosophy, Art, and Science of Chemistry* (Oxford: Oxford University Press, 2012).

¹¹ Roald Hoffmann, "Under the Surface of the Chemical Article." In ibid., 149.

other place where narrative is rife is in the hypothesis-forming stage of doing science.¹²

and:

Try writing an article with just the facts, and see how many people read it!...a world without stories is inhuman. It is a world where nothing is *imagined*. Could a chemist be creative in such a world?...There is another very human literary activity. This is to write poetry, to tell essences intensely, in words.¹³

In like vein, Part Two of *The Same and Not the Same* ("The Way It Is Told") collects several essays on the writing of scientific articles and related matters, introduced with:

Scientists have a nicely ambivalent attitude to the way their stories are told. On one hand, language is presumed immaterial — we supposedly have learned we need report the facts and nothing but the facts. Unambiguous mathematical equations and chemical structures make the story crystal clear, wherever on this globe it be told. On the other hand, the language (whatever language we speak or write) is all we have. With it, written and spoken, we must convince the world that the knowledge we have gained with so much labor and ingenuity is indeed reliable.¹⁴

The word *story* is key here: Roald sees the acts of presenting scientific findings and narrating a tale as, at their core, not different in any fundamental way. I appose here a comment from Susan Haack, a "traditional" philosopher of science, with whom I expect Roald would find scant agreement:

Rorty writes that he "views science as one genre of literature," or, he continues, "put the other way around, literature and the arts as inquiries, on the same footing as scientific inquiries." The idea of chemistry or astrophysics as genres of literature is nothing short of laughable. Even the idea of chemical reports, or the proceedings of astrophysical society, as genres of literature is pretty strange (though they are, to be sure, kinds of writing, as are bus timetables, and could be read somewhat as one reads literature — as one might notice happy alliterations or rhymes in the bus schedule).¹⁵

Indeed, Roald's view of the centrality of storytelling seems to me to have guided the way he chose to put *The Same and Not the Same* together. While I certainly would not say it is disorganized in any way, there is an ongoing feeling of having evolved naturally, rather than being governed by any tightly pre-imposed logical structure. Each story calls up the next, by connective association —working in somewhat (but not exactly) the same way as cognition:

¹² Roald Hoffmann, "Why Buy That Theory?" In ibid., 16-17.

¹³ Roald Hoffmann, Vladimir I. Minkin, and Barry K. Carpenter, "Ockham's Razor and Chemistry." In ibid., 74-75.

¹⁴ Hoffmann, *The Same and Not the Same* (above, n. 4), 55.

¹⁵ Susan Haack, "As for That Phrase 'Studying in a Literary Spirit..." *Proceedings and Addresses of the American Philosophical Association* 70, no. 2 (1996): 70.

I think chemistry is interesting...because its activities parallel deep avenues in our psyche — which I prefer to see not as a branching tree of neurons, shaped by genetics and experience (and chance), but as a completely interconnected multidimensional volume. In which a given fact (a molecule, a line from a poem) has a history, a context, to be sure. But it comes to life only if we think of the molecule (or the poem) as suspended — yes, tensely — in a space that is defined by different themes or oppositions.¹⁶

For example, Part 3 "Making Molecules" moves smoothly from Goethe's novel *Elective Affinities*, to the biosynthesis of a complex biomolecule (uroporphyrinogen-III), to an essay on what poets do, to the chemical synthesis of a deceptively simple molecule (cubane), to the Aganippe fountain, a work by Swedish sculptor Carl Milles, to an excerpt from Tchaikovsky's opera *The Queen of Spades*, and so on. This approach is well suited to appeal to the non-technical reader; at the same time, it self-manifests the importance of narrative in discourse, scientific and otherwise.

In the piece quoted above, Haack goes on to argue for a hard separation between literature and science, based in considerable part on the desirability of univocality:

But the fact that novelists, etc., engage in historical, geographical, psychological,..., philosophical inquiry... is no more a threat to the distinction between philosophy and literature than it is to the distinction between geography and literature....it is better to talk, not in terms simply of clarity and rigor (to which literary, no less than scientific writing aspires, but in a different way), but of *explicitness, directness,* and *univocality* (the qualities peculiarly desirable in scientific, and philosophical writing).¹⁷

whereas in essays co-written (collaborations with artists, writers, other chemists, *etc.* have been a hallmark of Roald's career, as I should have pointed out earlier!) respectively with fellow chemist Pierre Laszlo (an occasional participant in SLSA) and philosopher/poet Emily Grisholz, Roald expounds on his *very* different view of the essentiality of directness and univocality:

Humans delude themselves with mental constructs projected upon reality. The puritans among us...push for our minds to handle abstractions only, as in mathematics....While we have a great deal of respect for such an inclination...we are not such purists ourselves....Our discipline is a curious mix of empirical observation *and* abstract reasoning....Students brought up on deductive logic have a hard time with chemistry!¹⁸

[T]here is no single correct analysis of the complex entities of chemistry expressed in a single adequate language, as various reductionist scripts require;

¹⁶ Hoffmann, *The Same and Not the Same* (above, n. 4), 256.

¹⁷ Haack, "As for That Phrase 'Studying in a Literary Spirit..." (above, n. 15), 66-68.

¹⁸ Roald Hoffmann and Pierre Laszlo, "Representation in Chemistry." In Kovac and Weisberg, *Roald Hoffmann* (above, n. 10), 177.

and yet the multiplicity and multivocality of the sciences...do not preclude but in many ways enhance their reasonableness and success....We understand the reality whose independence we honor as requiring scientific methods which are not univocal and reductionist precisely because reality is multifarious, surprising, and infinitely rich.¹⁹

These quotes, to my mind substantially erase any border between literature and science.

Indeed, in yet another essay, Roald tells of a disagreement he had with a physicist over whether an as yet unknown form of carbon, which he had calculated would be unstable relative to known forms, might possibly be synthesized. The argument turned on their different intuitive understanding of the meaning of "unstable," which for Roald illustrated how much scientific thought is influenced by words and language rather than mathematical rigor:

In science, we think that words are just an expedient for describing some inner truth, one that is perhaps ideally represented by a mathematical equation....Yet words are all we have, and all our precious ideas must be described in these history- and value-laden signifiers....In fact, the more important the argument is to us, the more we want to be convincing, the more likely we are to use simple words. Those words, even more than technical terms, are unconsciously shaped by our experience — which may not be the experience of others.²⁰

There seems to me to be a substantial meta-argument in this piece (I don't know whether it might have been in Roald's mind while writing): the word "unstable" invokes not only the scientific issue but also the instability of meaning in all discourse, another facet of the inseparability of science and literature.

I include the fourth of Roald's major books, *Old Wine New Flasks*,²¹ along with his poetry and plays, under the heading of (for want of a better term) creative writing. (Of course creativity is ubiquitous in his essays — for that matter, also in his scientific work, as emphasized in quotes cited above.) This collaboration (another one!) with self-described "lapsed engineer" and essayist Shira Leibowitz Smith explores connections between science and themes from Jewish tradition by means of an eclectic mix of genres: two extended epistolary discussions (one by email, the other old-fashioned snail mail), a play, a (fictionalized) trial transcript, a couple of dialogues, etc. As an illustration, I've picked out one (more or less at random), which originates in a discourse on the importance of *chirality* — the property whereby many chemical compounds, especially biologically important one, exist in two non-identical mirror image forms — left- and right-handed "enantiomers."²² (This topic also features prominently in the first two books mentioned earlier). Shira calls to Roald's attention a passage from Deuteronomy that

¹⁹ Emily R. Grosholz and Roald Hoffmann, "How Symbolic and Iconic Language Bridge the Two Worlds of the Chemist." In ibid., 223.

²⁰ Roald Hoffmann, "Unstable." In ibid., 39.

²¹ Roald Hoffmann and Shira Leibowitz Smith, *Old Wine New Flasks: Reflections on Science and Jewish Tradition* (New York: W. H. Freeman & Co., 1997).

²² Roald Hoffmann and Shira Leibowitz Smith, "You Must Not Deviate to the Right or the Left." In ibid., 79-121.

concludes "you must not deviate from the verdict that they announce to you either to the right or to the left" and comments "I wonder if they had chirality in mind," provoking the exchange:

[Roald] I still say you're way out, Shira — why bring in stereochemistry (several millennia in the future), when all these guys are doing is using a metaphor?

[Shira] Sure, Rashi is expanding the biblical metaphor. But it's in the nature of talmudic and post-talmudic debate that everything is real, and everything is at the same time metaphorical ... and sometimes anachronistic. Or to put it another way, the discussion may be about obeying the courts, but it is also about chirality....It seems to me that the story of chirality is full of people telling each other that left is right!²³

The chapter goes on, at considerable length, to accounts of the development of chirality in chemical history, episodes of talmudic exegesis where "questions of left and right are never far away," analysis of paintings by Dutch artist Adriaen van der Werff (on a theme from Genesis) and Russian-Jewish artist Marc Chagall, and much more.

Of Roald's (three) published plays, by far the best known is *Oxygen*,²⁴ yet another collaborative effort with (now deceased) organic chemist Carl Djerassi; it has received a number of productions worldwide (the official premiere was in conjunction with an American Chemical Society national meeting in San Diego in April 2001, where I had the opportunity to see it). Its premise is that the Nobel Foundation has decided to institute a new program of "retro-Nobels," recognizing work done before the establishment of Nobel Prizes at the beginning of the 20th century. A committee for the retro-chemistry award quickly zeroes in on the discovery of oxygen as a worthy subject for the award. But who should receive it? Carl Wilhelm Scheele, a Swedish pharmacist, who was apparently the first to obtain a sample in the laboratory? Joseph Priestley, the first to publish his findings? Antoine Lavoisier, the first to understand what oxygen really is? All three?

Science-themed plays (of which there have been many, especially in recent years²⁵) face a challenge — at least some of the scientific content must be accessible to a general audience for the play to work — which is acknowledged in *Oxygen*, in effect, by one of the committee member characters: "Who'd like to come up with some simple phrases to explain to [the] public that without the discovery of oxygen there would've been no Chemical Revolution ... no chemistry as we now know it?"²⁶ In particular, the debate centers on the historical background: Lavoisier was the first to understand the role of oxygen in phenomena such as combustion and rusting, thereby overthrowing the phlogiston theory in which both Scheele and Priestley devoutly believed. Unless one appreciates the significance of that, the priority dispute makes little sense. On the other hand, one of the more basic rules of theatre is "show, don't tell." How can the

²³ Ibid., 86.

²⁴ Carl Djerassi and Roald Hoffmann, Oxygen: A Play in Two Acts (Weinheim, Germany: Wiley-VCH, 2001).

²⁵ Kirsten Shepard-Barr, *Science on Stage: From Doctor Faustus to Copenhagen* (Princeton, NJ: Princeton University Press, 2006).

²⁶ Djerassi and Hoffmann, Oxygen (above, n. 24), 28.

essential content be effectively communicated without violating that rule, descending into didacticism, and risking a complete breakdown of rapport?

To (partially) solve this problem, Djerassi and Hoffmann make use of a device that has featured in other science-themed plays, most notably Tom Stoppard's *Arcadia*. The action shuttles back and forth between two time periods: a (fictional) 1777 meeting of the three chemists, invited to Sweden by then-King Gustav III to decide who should get credit; and the contemporary deliberations of the committee, whose arguments in favor of their candidates echo not only those made by the candidates on their own behalf but also stories about priority claims and professional jealousy among themselves. The resonance between the two is nicely reinforced by having a single actor play each candidate-advocate pair (temporal scene shifts are signaled by minor costume changes), as well as the inclusion of a young historian of science writing her dissertation on "Women in the lives of 18th century scientists" as secretary to the Nobel committee (the wives attend and play important roles at the 1777 meeting, especially Mme. Lavoisier). Some of the chemistry is presented in the form of a stylized masque, "The Victory of Vital Air Over Phlogiston," performed by the Lavoisiers.²⁷

Near the end, a committee debate addresses the similarities/differences between literature and science:

[Sune] You're pushing for a consensus, when we should be making a tough choice: one winner only. Take the Literature Nobel. It's never shared!

[Ulf] You're ignoring two fundamental differences between literature and science. The literati don't worry about priority ... and if they had a retro in Literature, it would've gone to Shakespeare or Dante or Cervantes ... or whoever ... but it wouldn't be shared. If Shakespeare had never lived, "King Lear" could never have been written. Without Dante, there would be no "Divine Comedy." Without Cervantes —

[Sune] Ulf, what's your point?

[Ulf] Simple! Consider oxygen. If Scheele or Priestley or Lavoisier had never lived, somebody would have discovered oxygen. The same with Newton and gravity, with Mendel and genetics —

[Sune] So why give a Nobel at all....If it would happen anyway, why worry who is first?

[Astrid] Science is done by scientists ... humans are competitive ... scientists are even more competitive ... and they want to be rewarded for being first.²⁸

Roald's poems, again, range widely in subject and style; many clearly were inspired by perceived connections between his scientific and extra-scientific life. One nice example,

²⁷ Ibid., 42-45.

²⁸ Ibid., 108-109.

"Theoretical Chemistry," portrays a common (and often difficult) problem in Roald's scientific field — trying to identify by calculation the most favored pathway followed in a chemical reaction — in much more mundane and familiar terms:

I would sit just there, in the quiet shade of the live oaks. It was a scholar's dream, but I, intent to find the way across the ravine, wasn't there to write poetry. You see, that thick lush growth stopped progress

here, but I could spot a road gathering on the other side. That's where we had to go. I brought my field glasses, a topographic map. From above, the gully looked much like a low-growing jungle hugging the land;

the cows had gotten across, I saw tracks in and tried to follow them. But it didn't work, bushes closed in, there was poison oak, vines with rows of sharp red thorns. I came back day after day, trying, tracing paths back

from the other side. For I knew a pattern, the right way, had to be there. In the end I found one, but what's bothered me since is that I didn't follow the paths that are hidden there, the way I should have, but

I hacked a rough piece of a new one through. The other day I met a friend who's run into the same wild terrain. Starting out from a hill nearby, he found a different way. But I told you there was only one.²⁹

Others relate the molecular motions responsible for heat to a jai alai game;³⁰ explain the technique of scanning tunneling microscopy by invoking erotic images,³¹ or that of optical spectroscopy from within the Mayan *Popol Vuh*;³² compare the elucidation of a chemical structure to creation of a sculpture in wood;³³ and many more.

²⁹ Roald Hoffmann, "Theoretical Chemistry." *Southwest Review* 95, no. 1/2 (2010): 207.
³⁰ Roald Hoffmann, "Heat: Hot As _____: Cold." In *Memory Effects* (Chicago: Calhoun Press, 1999), 36.

³¹ Roald Hoffmann, "The 1986 Nobel Prize in Physics." In *ibid.*, 46.

³² Roald Hoffmann and Pierre Laszlo, "The Say of Things." In Kovac and Weisberg, Roald Hoffmann (above, n. 10), 197-198.

³³ Roald Hoffmann, "The Difference Between Art and Science, II." Webster Review 14, no. 2 (1990): 89.

The first piece in *Old Wine New Flasks* is an exchange of letters between Roald's coauthor Shira Leibowitz Smith and a young woman, Ayyal (a relative? It isn't made clear), who has put her plans for a scientific career on hold while wrestling with her concerns that science is antithetical to Nature. Shira suggests inviting Roald into the conversation; Ayyal agrees, though with the caveat "Those chemists are the worst; their labs and factories are to blame for this incredible pollution we have." But after reading his first letter, which problematizes any distinction between natural and man-made, she comments "Are you really a chemist? You don't write like one."³⁴ As a chemist myself, I would hate to think that the way a chemist writes is necessarily diametrically opposite to the many illustrations we have seen here, although I certainly see her point. But perhaps things can improve. In his comments accepting the SLSA Lifetime Achievement Award, Roald mentioned that among his ambitions, he wants to help likeminded scientists to "come out of the closet," to legitimize their desire to follow their passions by providing a prominent example of one who followed his. Perhaps those efforts could help us succeed in attracting more scientists to SLSA.

³⁴ Roald Hoffmann and Shira Leibowitz Smith, "Is Nature Natural?" In Hoffmann and Leibowitz Smith, *Old Wine New Flasks* (above, n. 21), 1-54.