Looking for Connections: An Interview with Roald Hoffmann

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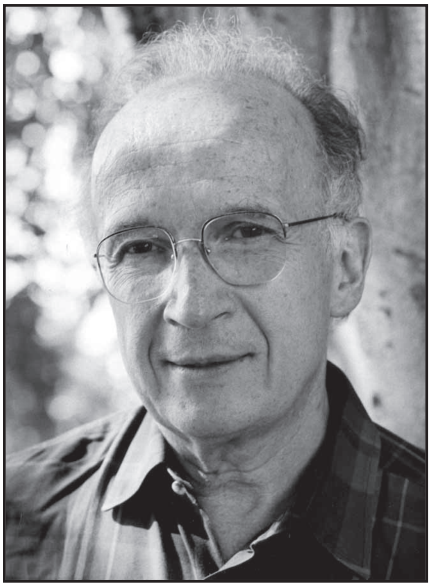
A Brief Biographical Sketch

Roald Hoffmann was born in Zloczów, Poland (now Zolochiv, Ukraine), in 1937, dark days in Europe. The happy home life he experienced with his Jewish family was short-lived, although he and his mother managed to survive the Nazi occupation. In 1946 he left Poland for Czechoslovakia, Austria, and Germany, finally arriving in the U.S.A. in February 1949, at the age of 11. He continued his primary education in New York City and graduated from Stuyvesant High School there in 1955. In the same year he became a naturalized citizen of the U.S.A. He entered Columbia College in New York as a Pulitzer Free Scholar and, in 1958, received his B.A., summa cum laude, majoring in chemistry.

Hoffmann's interest in chemistry developed during the summers of his college career while working at the National Bureau of Standards with E. S. Newman on the thermochemistry of cement compounds and with R. E. Ferguson on the pyrolysis of hydrocarbons. Then he began graduate study at Harvard University in 1958, obtaining a M.A. in physics in 1960 and a Ph.D. in chemical physics in 1962. His thesis work was completed under the joint supervision of Martin Gouterman and William N. Lipscomb and dealt with the molecular orbital theory of polyhedral molecules.

In 1962, he was elected a Junior Fellow in the Society of Fellows of Harvard University and he remained in this position until 1965. During this period he began work on the electronic structure of organic molecules. At the end of this stay at Harvard, he began his collaboration with Robert B. Woodward on the theory of concerted reactions.


Roald Hoffmann (photographed by Clemens Loew).

In 1965 Hoffmann joined the Department of Chemistry at Cornell University as associate professor of chemistry. In 1968 he was appointed professor of chemistry in the same department, and in 1974 he became the John A. Newman Professor of Physical Science. Since 1996 he is both the Frank H. T. Rhodes Professor of Humane Letters and a professor of chemistry; almost every year he has taught first-year general chemistry.

Hoffmann received the 1969 American Chemical Society Award in Pure Chemistry and the 1970 Award of the International Academy of Quantum Molecular Sciences. In 1973, jointly with R. B. Woodward, he received the first Arthur C. Cope Award in Organic Chemistry from the American Chemical Society. In 1981 he shared the Nobel Prize in Chemistry with Kenichi Fukui "for their theories, developed independently, concerning the course of chemical reactions". In 1982 he received the ACS Award in Inorganic Chemistry and in 1990 he received the Priestley Medal of the American Chemical Society, its highest honor. In 1991 he received the first (and last) Gold Medal in honor of Russian chemist N. N. Semenov, awarded by the Academy of Sciences of the USSR. In 1996 he received the Pimentel Award in Chemical Education from the American Chemical Society. In 1997 Hoffmann received the first Elizabeth A. Wood Science Writing Award of the American Crystallographic Association; in 1998 he received the Jawaharlal Nehru Birth Centenary Award of India. In 1999 he was made an Honorary Member of the German Chemical Society.

Hoffmann is fascinated by and interested in everything from philosophy to visual arts and poetry. He is an accomplished artist as well as a scientist. At Columbia he was introduced to poetry, and through the years he maintained an interest in literature, particularly German and Russian literature. He began to write poetry and published his first poem in 1984. His first poetry volume, *The Metamict State (1),* was published in 1987; *Gaps and Verges (2)* followed in 1990, and *Memory Effects (3)* was published in 1999. Hoffmann's poems are characterized by metaphors and intense images, many drawn from scientific ideas and concepts.

His most recently published collection is *Soliton (4)*. In 1993 the Smithsonian Institution Press published *Chemistry Imagined,* a unique art–science–literature collaboration of Roald Hoffmann with artist Vivian Torrence. In 1995, Columbia University Press published Hoffmann's *The Same and Not the Same (5).* In 1997, W. H. Freeman published *Old Wine, New Flasks: Reflections on Science and Jewish Tradition*, by Hoffmann and Shira Leibowitz Schmidt *(6, 7).* He is author with Carl Djerassi of the play *Oxygen (8, 9),* which premiered in the U.S. at the San Diego Repertory Theatre in 2001, and, on his own, of a new play (2006), *Should've (10).* In 1986–1988 Hoffmann participated in the production of a television course in introductory chemistry entitled "The World of Chemistry" *(11).*

Hoffmann's chief contribution to chemistry continues to be the actual blending of computations stimulated by experiment and the construction of generalized models, of frameworks for understanding. In more than 500 scientific articles and two books he has taught the chemical community new and useful ways to look at the geometry and reactivity of molecules, from organic through inorganic to infinitely extended structures.

We are about to meet a multifaceted man with extremely rich mental capacities and ethical values. The aim of this interview it to convey to readers some flavor of his unique blend of science, art, and humanity.

Hoffmann kindly agreed to be interviewed and what follows is a conversation between him and the author.

Tough Beginnings

Liberato Cardellini: Let us begin with your name. Why are you called Roald Hoffmann?

Roald Hoffmann: I was named Roald after the Norwegian polar explorer, Roald Amundsen. He died 10 years before I was born, but there was an article in the newspaper about him that my parents read and they gave me his name. I was born as Roald Safran. My father was killed by the Nazis in 1943. After the war my mother remarried, and I took my stepfather's surname and became Roald Margulies. Then, on the way out of Poland, we bought the documents of a dead German named Hoffmann and I adopted that name. It was easier to enter the U.S. with German nationality, rather than Polish. Such is life!

In your life you have experienced the greatest and the darkest moments of the human soul. Can you recall some of the persecutions you had to suffer for the moral stance of the new generations?

I lived through very dark times—my father, three of my grandparents, and several aunts and uncles were killed. My mother and I survived, but we did not survive because we were better human beings. We survived by chance, because of my parents' political (socialist) awareness. And because we were helped by one good man. It is so sad to think of how many lost their lives. Of the 4000 Jews in Zloczów, where I was born, perhaps 200 survived the war, five children among them.

Is it possible to find an explanation for human nastiness? How can you make sense of sorrow?

Ah, Liberato, those are the questions. And science is of no help in answering them. There is no "solution" to sorrow. Only an infinite, shifting set of resolutions, in which the thousand and first "answer" has as much validity as the thousandth one. And poems provide some of the best resolutions.

Becoming a Chemist

You are a theoretical chemist. Who inspired your love for organic chemistry? Why does "Making Molecules" put chemistry very close to the arts?

I liked organic chemistry from the moment I encountered it at Columbia College. But it was only the collaboration with R. B. Woodward that made me realize the beauty of this intellectual construction, both structure and synthesis.

As for your second question, chemists make molecules, by hard work, clever construction, and chance. They create, subject to some governing rules, something new, often something that has not been on Earth before. And then they study their creation, see its properties and relationships. They contemplate it. And they go on to make more molecules. I think the process is much like art. But there are differences.

What has been the meaning of the laboratory in your experience as a student and teacher?

As a student I was pretty good at labs. I loved the physicality of blowing glass and of solutions changing color. I liked the existentialist moment of getting a qualitative or quantitative analysis of an unknown.

Teaching Chemistry

As a general chemistry teacher, what are the most important things you hope to instill in your students?

That chemistry is about change; that there is nevertheless an equilibrium, yet an equilibrium that can be disturbed. That the natural world is complicated, for good reasons, although we can live with that complexity.

As researchers we have long training in labs. As teachers, a much more demanding profession, we learn the skills as we go along. Why are teaching and learning not taken seriously (12)?

I think it is taken seriously. We learn from our mistakes (in science, not in love). And if we are good teachers, we learn to listen, at least in part, to what our students tell us. So, for instance, we want them to see the relationships between the various parts of chemistry and this world and they tell us that they want just to know what will be on the exam. The middle ground is that compartmentalization is not a bad strategy for learning, or building automobiles, or running a eukaryotic cell. Still there is a time to be human, which means to pass beyond compartmentalization, to see the connections that make life interesting.

How can chemistry help in solving the problem of pollution?

By developing methods of "green chemistry" that avoid waste, that are economical in atoms and energy and which use environmentally friendly solvents.

Chemical Research, Past and Present

What is your "research style"? What is the question you are researching into now?

My research style is to go into details, not to move toward a general goal or to work on problems perceived as important. As I go into details, I keep my eyes open for connections and often they are there *(13–15).*

I am working right now with great joy on trying to understand the complex structures that molecules assume at high pressures, and the place a chemical intuition has in these. I'm also interested in designing variants on the Bergman rearrangement, a fascinating chemical reaction, and in designing some new metallic structures.

You have researched in all branches of chemistry; you have received ACS's prestigious A. C. Cope Award in Organic Chemistry jointly with R. B. Woodward, as well as having received the Society's Inorganic Chemistry Award. What's your secret?

First of all, I'm interested in everything. Secondly, I was lucky—I had a theoretical method that allowed me to do calculations on any molecule under the sun. With this method we could do organic molecules and inorganic ones. Third, I had the kind of personality that was not bothered by that theoretical method not being always right nor mathematically rigorous. And then I learned solid state physics, and saw that the language of orbital interactions could also be used to understand bonding on surfaces and in solids. The underlying thread is that the chemical world is connected.

Representing Chemical Ideas

Atomic orbitals are just mathematical constructs and some of us—myself included—teach orbitals without having a proper knowledge of quantum mechanics. From the time of The Conservation of Orbital Symmetry (16) *you have done a lot of work with orbitals. What ideas of orbitals should we teach so that they need not be untaught later? How do you teach this topic?*

I think orbitals are real, and from orbitals we can build the world of chemistry. They are the most far-reaching and unifying way to see chemical phenomena. They also have a curious graphical affinity with the structural formulas of chemistry and, once they have been learned, they somehow suit the geometric intuition of the chemist.

Erwin Schrödinger wrote: "Every man's world picture is and always remains a construct of his mind and cannot be proved to have any other existence" (17). *In chemistry we use formulas: what do chemical formulas represent? How much do they resemble reality?*

There are layers of representation, each with their own utility. Formulas are all we need to do stoichiometry. Chemical structures give connectivity, what is bonded to something else. Then there are the primitive graphics and models that we use to communicate essential three-dimensional shape. There is an underlying reality with many representations of it.

You see beauty in the structure of molecules and you talk about "unexpected desymmetrization of the beauty (Platonic and Brazilian) of buckminsterfullerene" (18). *In what sense did awareness and appreciation of aesthetics lead to discovery* (19)?

Actually my feelings about aesthetic criteria in science have evolved, from a position where I was drunk, in a way of speaking, on symmetry and simple explanations, toward a place where I now think that aesthetic criteria may sometimes be overly seductive. The problem is that the aesthetic criteria with which we are born favor simplicity, order, symmetry, probably for some good evolutionary reason. Politicians capitalize on our desire for simplicity. But the world is not that way. It is often complex, disordered, unsymmetrical like a ribosome, rather than like cubane, a molecule that I love. Our problem is how to see the beauty in complexity, in our lives, and in nature. Beauty resides at some tense edge where simplicity and complexity, order and chaos, contend with each other.

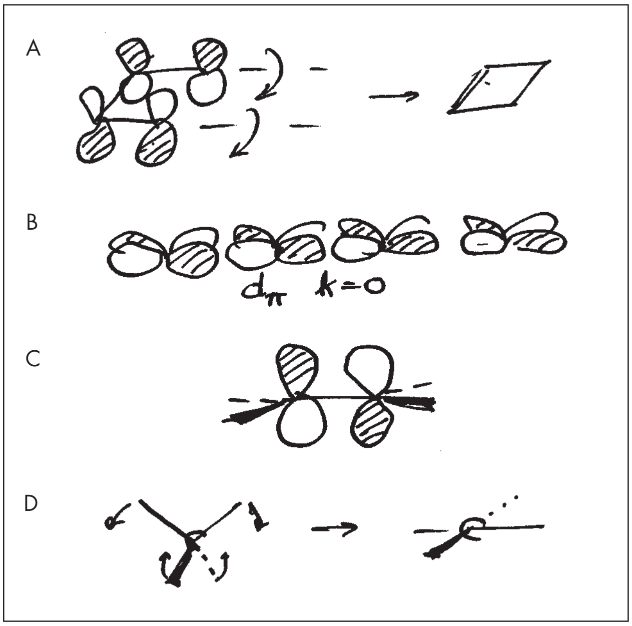


Figure 1. Reactions drawn by Roald Hoffmann. (A) Conrotatory cyclization of butadiene to cyclobutene. (B) A crystal orbital in a chain of transition metals. (C) The π^* orbital of ethylene. (D) Transforming tetrahedral methane into square planar methane.

Your numerous papers are filled with drawings and formulas. Could you write the reactions you are most proud of and tell us about them?

The top one (see Figure 1A) is the controlling frontier orbital in the conrotatory cyclization of a butadiene to a cyclobutene—so an evocation of my fruitful collaboration with R. B. Woodward. Below it (see Figure 1B) is a chain of d orbitals in a linear metallic array—this time referring to something I am proud of, having taught chemists not to be afraid of solid state physics. Next (see Figure 1C) the π^* orbital of ethylene, important in its bonding to a transition metal, in organometallic complexes. And at the bottom (see Figure 1D), a motion that takes tetrahedral methane into square planar—the unthinkable worth thinking about.

Philosophical Beliefs

In what sense is circular reasoning useful in chemistry?

I would call it "nearly circular reasoning". It helps one to get support for a hypothesis and encourages one to go on.

It is also consistent with what I call horizontal thinking: that is, defining concepts in terms of words or other concepts at the level of questions asked in the field. For more on this, see my struggle with reductionism in Chapter 4 of *The Same and Not the Same (5)*.

The logic of chemistry is not mathematical logic. We often reason in ways that are productive, that build support for a theory and suggest experiment. But examined in detail, the logic may be faulty. So we talk of oxidation states, even though we know that they are not real charges on an atom. We often construct rationalizations, stories that explain why something is one way or another, and then talk about them as predictions. The nearly circular thinking builds confidence, even if it is imperfect thinking. It gives one the incentive to try an experiment *(20).*

What is it wrong with reductionism?

Reductionism is a definition of what constitutes satisfactory understanding. A hierarchy of sciences is set up, and understanding is defined in terms of reduction to the science "below" and so we consider biology in terms of chemistry or chemistry in terms of physics. This is pretty silly, not representing reality, nor the way science is really done.

I think there are at least two kinds of understanding; vertical, which is reductionist, and horizontal, which is understanding a phenomenon in terms of a set of concepts, experimental and theoretical, of the same complexity as the object one is trying to understand. So a poem is vertically understood in terms of the firing of neurons in the author's mind and the reader's mind, but infinitely more interestingly, in terms of the psychology of the people involved and the language they use. Most of the concepts that move chemistry forward—such as the idea of a chemical bond, functional groups, aromaticity, acids and bases—are horizontal ways of understanding, quasi-circular in their logic, not reducible to physics, and yet tremendously productive. These chemical concepts are less interesting when one tries to reduce them to physics.

Primo Levi—the Italian chemist who dedicated himself to revealing to the world the Nazi atrocities—was, like you, a writer and a poet. What do you think makes Levi great: his depression, his reserve, his suffering, or what?

What makes Levi great is his desire to see in chemical fact a metaphor for the human condition, and his talent for expressing that in words for others to appreciate.

Are there analogies between your teaching and your poetry?

In both, I try to understand the world. Both also speak out, to people. That is why I want to share my understanding, I want to show someone what is beautiful about the way a vibrating CO_2 molecule heats up the oxygen and nitrogen molecules of the atmosphere (the last step in greenhouse warming). An economical way of explaining something creates intensity. This is present in the best poetry and in good teaching. Though repetition has pedagogical value, it is less valuable in poetry except as a reinforcing, rhythmic device.

You accept Ockham's Razor (21)*—the metaphysical assumption that the world is simple—yet you contend the reductionist idea. Why is this not a contradiction?*

Actually, I dislike Ockham's razor intensely. It is a device that limits the imagination and tends to cut interesting stories short. Too many people apply Ockham's razor as they construct hypotheses; but they should apply it later, and meanwhile weave hypotheses that are as imaginative as possible. Ockham's razor also works best within a reductionist framework, whereas I believe that science progresses in definitely unreductionist ways.

A final and more personal question: You defined yourself as "an atheist who is moved by religion" (6). *Looking at the tenor of your life and the many goals you have achieved, one wonders where your inner force comes from.*

The atheism and the respect for religion come form the same source. I observe that in every culture on Earth, absolutely every one, human beings have constructed religious systems. There is a need in us to try to understand, to see that there is something that unites us spiritually. So scientists who do not respect religion fail in their most basic task—observation. Human beings need the spiritual. The same observation reveals to me a multitude of religious constructions—gods of nature, spirits, the great monotheistic religions. It seems to me there can't be a God or gods; there are just manifestations of a human-constructed spirituality.

I also found that I respond to ritual, be it of a Catholic Mass, the synagogues that are part of my Jewish background, or Afro-Brazilian possession rites. But that is not where my inner force comes from. It comes from survival and the joy of life. It comes from the struggle of trying to understand the world; beautiful and terrible as it is and seeing that everything is connected to everything else.

Some Final Words

Considering his success in fulfilling the many roles of scientist, teacher, poet, philosopher, and writer, it is a privilege to have Roald Hoffmann as a member of our chemistry community.

These Web sites of Roald Hoffmann, at *http://www.roaldhoffmann.com/pn/* and *http://hamiltonian.chem.cornell.edu/* (both accessed Jul 2007), provide an overview of his scientific work and display some of his other works and projects, as well. To reach excellence in science and art can be a very difficult task for anyone, although not (it seems) for Roald Hoffmann *(22):*

> I have no problem doing (or trying to do) both science and poetry. Both emerge from my attempt to understand the universe around me, from my own personal affection for communicating, teaching what I've learned, and from my infatuation with language—the English language, as well as other languages that geopolitical accidents have thrust into my head. ...The creative act is cross-cultural and inherently altruistic.

> Both science and art also share elements of a common aesthetic. ...Ultimately, the common ground is a shared, complementary struggle to comprehend what is in and around us.

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