Living Joyfully with Complexity in Chemistry and Culture

Roald Hoffmann

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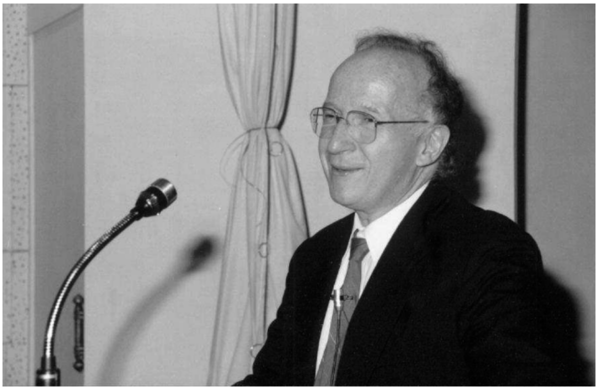

Fig. 1. Roald Hoffmann delivering the B.M. Birla Memorial Lecture

Roald Hoffmann was born in Zloczow, Poland in 1937. Early in life, he had to face persecution from the Nazis. He however managed to escape with his family and arrived in the United States in 1949. He graduated from Stuyvesant High School, Columbia University and obtained his PhD in 1962 from Harvard University, working with W.N. Lipscomb and Martin Gouterman. After a brief stint at Harvard as a Junior Fellow from 1962 to 1965, he joined Cornell University where he has been the Frank H.T. Rhodes Professor of Humane Letters and Professor of Chemistry.

Professor Hoffmann is a member of the United States National Academy of Sciences, The American Academy of Arts and Sciences, and the American Philosophical Society. He has been elected a Foreign Member of the Royal Society, the Indian National Science Academy, the Royal Swedish Academy of Sciences, the Finnish Society of Sciences and Letters, the Russian Academy of Sciences and the Nordrhein Westfallische Academy of Sciences. He has received numerous honors, including the Life Time Achievement in Science

B.G. Sidharth (ed.), *A Century of Ideas,* 101–108.

Award of the B.M. Birla Science Centre and over twenty five honorary degrees. He is the only person ever to have received the American Chemical Society's awards in three different specific subfields of Chemistry – the A.C. Cope Award in Organic Chemistry, the Award in Inorganic Chemistry, and the Pimentel Award in Chemical Education, as well as two other ACS awards. In 1981, he shared the Nobel Prize in Chemistry with Kenichi Fukui.

In more than four hundred and fifty articles and two books Professor Hoffmann has thrown a new perspective to look at the geometry and the reactivity of molecules from Organic to Inorganic to infinitely extended structures.

In recent times Professor Hoffmann has looked at the electronic structure of extended systems in one, two, and three dimensions. Frontier orbital arguments find an analogue in this work in densities of states and their partitioning. An especially useful tool, the COOP curve, has been introduced by the Hoffmann group. This is the solid state analogue of an overlap population, showing the way the bond strength depends on electron count. The group has studied molecules as diverse as the platinocyanides, Chevrel phases, transition metal carbides, displacive transitions in NiAs, MnP and NiP, new metallic forms of carbon, the making and breaking of bonds in the solid state and many other systems. One focus of the solid state work has been on surfaces, especially on the interaction of CH4, acetylene and CO with specific metal faces. The group has been able to carry through unique comparisons of inorganic and surface reactions.

He is a multi-dimensional character. Not just a research scientist, he has also been involved in pedagogy and popularization. He participated in the production of a television course on Chemistry. This twenty six episode series was developed at the University of Maryland. Professor Hoffmann was the presenter and narrator of the series. He has also written popular articles as well as thought provoking articles on Science and even the Arts including poetry. In fact in 1993 the Smithsonian Institution Press published "Chemistry Imagined" which was a collaboration with artist Vivian Torrence on Art, Science and Literature. A play, "Oxygen" written with Carl Djerassi had its premier at the San Diego Repertory Theatre in 2001 and had productions at the Riverside Studios in London and Wurzburg and Munich for the German version, in the fall of the same year. This play has been broadcast by BBC World Service and West German Radio and has been published in English and German translations. These are but a few examples of Professor Hoffman's versatility.

He is a very humane person. This trait has undoubtedly been enhanced by his traumatic experience in the Nazi period. In conversation he described at length his escapade, using false names and passports. It is nothing short of a real life thriller. His great love for students and the amount of time and patience he can devote to them is also very touching, as was demonstrated at Hyderabad. He not only patiently gave his autographs to the huge crowd of students, but also illustrated each autograph with one of his typical chemical diagrams.

Though soft spoken, Professor Hoffmann is also outspoken. He said that if he were to meet the Prime Minister (of India), he would tell him that rather than all the esoteric research which is going on in the laboratories, India should tie up with a country like Columbia to develop a much needed malaria vaccine. He added that such a vaccine could be developed in about six months in the United States, but it won't happen for all the wrong reasons. Malaria is a third world disease and there isn't enough money to be made out of such a vaccine.

I am pleased to be in the B.M. Birla Science Centre, at the invitation of Dr. B. G. Sidharth. The Birla Science Centre is dedicated to the widest possible dissemination of knowledge. I am very pleased to be here because I myself believe that we as scientists must be dedicated in the widest possible sense to talking about science to the general public, not only to our students and future colleagues and competitors in science.

There are many reasons for speaking about science to the general public. One motivation could be to attract more people to our profession. More important is that it is impossible for a democratic society such as India to function without the broadest possible awareness of some of the basic ideas of science by the general public. Scientists form only about one percent of our population. Research is possible only when the other 99% of society understand what scientists do. People ultimately make the decisions. They may seek the advice of experts, but experts can be martialled on the side of any issue in the world. It is important that people themselves learn at least some basic ideas of science, so that they can judge the words of experts and listen to them critically, as well as to the words of politicians. It is very important for the functioning of a democratic society that people know about science.

There is another reason, a psychological one. If we do not know how the world around us works, we create, in the tradition of human beings over ages, mysterious explanations and superstitions around the workings of that world. In the old days those things were created around the motion of the planets, around eclipses, comets and other phenomena – what is interesting today is that science and technology have surrounded us with all kinds of things that we don't understand. Do you know what goes on inside a CD player or inside your modern automatic camera? Those mysteries can well separate us from the things that we use, and so soon we are alienated, in the psychological sense, from the world around us.

It is in the spirit of this that I would like to tell you, speaking very much to the young people in the audience and to people who are not at all in my profession, something about chemistry. But what I will tell you about chemistry is not what you will see in a normal textbook. It is a kind of reflection on chemistry or an examination of several cross sections of chemistry.

Chemistry may not sound interesting, because it is in the middle. We don't have the infinitely big and we don't have the infinitely small, we only have a piece of life. But the word interest, if you look at its etymology, comes from the Latin (and then eventually probably from the Sanskrit) inter-esse; "inter" is between and "esse" is to be in Latin. So to be in between is to be potentially interesting. The cosmology of galaxies and the nature of elementary particles will not create a new pigment in a dye. You worry about whether a certain molecule can affect you or not because the molecule is on the scale of molecules in us. Chemistry is interesting. It is in the middle, it is on the human scale, it concerns people.

The first description of chemistry, the first of at least three that I would give you, is one that could have been given five hundred years ago. Chemistry is the art, craft and business of substances and their transformations. This definition predates science. I assure you there was chemistry, not only in our bodies, but chemistry done by human beings, before there was science. Let me give you two examples just from the culture around you – Tapioca/manioc is a substance that has to be processed by boiling in order to remove a poisonous substance in it before it can be eaten. That is chemistry. One of the most beautiful and useful dyes in world culture is indigo. Before people even learned how to make indigo in the laboratory that material was processed from a plant of the pea family and made into a beautiful dye in most tropical cultures. People processed manioc and indigo without waiting for chemists and laboratories, learning from many years of experimentation.

In order to show you the essential transformation at the heart of chemistry, what I would need to do is an experiment, because that is the heart of chemistry. It is some sort of change in some substance, but I did not know if I could do an experiment here. For example let us take a bromine and aluminum. If we put aluminium into bromine absolutely everything that you expect of chemistry takes place – foul odors, smoke, fire, if not an explosion. This is change before your eyes, from the reddish brown liquid bromine and the beautiful silvery metal of aluminium we get an aluminium bromide which is a white powder. This shows what chemistry is about.

The changes that take place are obviously not always so violent or quick as this one. If a neighbor next to you is awake (or alive, even if he is not awake), he is a wonderful example of chemistry at work. Proceeding much more slowly and much more quickly than the reaction we've seen, the enzymes in our bodies are transforming other molecules at the rates of millions of molecules per second. There are vast changes going on in us. Our kidneys, for instance, are processing a pound of bicarbonate every day. Incredible chemistries are taking place within us.

One interesting consequence of chemistry being about substances and their transformations is in a perception of chemistry that follows. In a comic book, Donald Duck comes in and says, "Hi what's cooking?" and his nephews say, "We don't know. We are playing with our chemical stuff." And then he says, "Why don't you pour this stuff in?" There follows the obligatory explosion, the necessary bump on his head. More interesting is the next panel, in which Donald suggest that the nephews mix CH_2 with NH_4. Peter Gaspar and George Hammond brought this strip to my attention; in a paper of theirs on CH_2-like molecules they simply said, "Some experiments on CH_2 suggested in the literature have not yet been tried." The reference was to Donald Duck's Walt Disney comics! Perhaps one of you can do it, it's not an easy experiment.

Consider next the Greek alchemical manuscript illustrating the principles of alchemy. Most scientists, especially chemists, have a rather ambiguous picture of alchemy. Alchemy was a philosophy associated with chemical experimentation that arose in a number of cultures – in China, in India, in Egypt, Greece and Europe in medieval times. In the manuscripts there is a picture of a swan that is biting its own breast and some oils in a chemical flask. In another Alchemical illustration, there is the wedding of a king and a queen by a bishop, but on the side, unlike any wedding that you have seen or are likely to see, people are doing chemical experiments. There is obviously something symbolic being communicated.

Many things came from alchemy: in Europe the making of the strong mineral acids, of sulphuric acid, nitric acid and hydrochloric acid; much of the shape of the glass vessels in alchemical illustrations is not that different from things that we see in a laboratory today. The philosophy of alchemy is change. What kind of change? The change of a sick person to a healthy person. The change of a base metal like lead, to a noble metal like gold. Perhaps a psychological change in a person performing the experiments themselves.

Modern scientists would like to take what the alchemists gave us. They would forget about the underlying philosophy. And laugh a little nervously at the kind of the dishonesty that inevitably accompanied something like making gold out of lead. I would say you can't do that – they are all tied together. What I think is interesting here is that the philosophy of change came first, when it wanted to get into people's souls and hearts, and looked around in the world for something which really represented a change of people – it found Chemistry. Chemistry was being used by a philosophy as a metaphor for change. This is very interesting.

There is a painting by a Dutch painter of 1570, Jan van der Straat. It is now in Florence, and it represents a late Alchemical Laboratory in the court of the Duke of Florence. It shows the patron Duke doing experiments in his newly commissioned laboratory. The woman in the center, holding a flask, is Bianca Capello, the second wife of the Duke. Behind him is a figure that would be recognizable to anybody here, and that is the Master Alchemist. He is the Director of the Laboratory. He is doing nothing, telling others what to do. Around them are figures doing all the work – the graduate students, as recognizable today as then.

This is a wonderful illustration of the eternal sociology of science. But there is a difference between 1570 and our times. When the Duke of Lawrence wanted to have himself, his wife, and his courtiers to be painted in an official portrait, a fun portrait to be sure but still an official one, he dressed up in the clothes of a chemist and did some chemical experiments. Can you imagine the President of the United States or the Prime Minister of India doing that today?

Now something has happened in the last two hundred years – we have learned to look inside the innards of the beast, where the substances are changing. It is in the nature of curious human beings to try to understand what happens when aluminium is placed into bromine and it changes in some way. We have developed the tools for looking inside matter. But something I must tell you right away, there are no microscopes to do this. You can't see molecules, except in some special circumstances. All of the beautiful structure of Chemistry was developed as a kind of knowing without seeing, slowly and laboriously formulated by human beings and their tools, building slowly a body of knowledge of what is inside. We now know that at the microscopic level in substances are atoms, and much more important than atoms – persistent groupings of atoms called molecules.

Chemistry is still the art, craft, business and now science of substances and their transformations. But it is also the same art, craft and science of molecules and their transformations. And any chemist today thinks both micro and macroscopically.

I want to represent some of these molecules for you. So I will show you some of them, some of the simplest possible ones that you can build from carbon or hydrogen atoms. At least two of them are quite familiar to us: Methane – this is the main component of natural gas. You also see propane, which is used in heating in various ways, and in between them, ethane. These are the three simplest hydrocarbons.

I have represented these molecules not in one but in three different ways, which are recognizable to you as a chemical structure, as a ball and stick model, and as something a chemist would call a space – fitting model. Why do I show them in three ways? This has something to do with the communication between scientists and people outside of science, especially people in the Arts and Humanities. You see, scientists have given the world the impression that they have a strangle hold on reality, that they really know what's in there and in the world. That is why TV ads or placards show men in white coats who are telling us what someone would like us to believe is true.

Now the reality is . . . that there is an underlying reality, there is a methane molecule, there is a propane molecule. But when I draw it, I am representing reality and communicating to someone else the nature of that molecule. I am very much engaged in representing things and ideas. And there isn't only one way to do that. Reality is objective, representation of reality is subjective – I choose the representation appropriate to the act of communicating my goals and intent, and to the receiver of my message. Sometimes I want to show the chemical structure, that is sufficient. And sometimes I am interested in the shape of the molecule. We do this in chemistry without thinking but it is important to realize how subjective our scientific representations are, because...people in the humanities and the arts are always representing things in many different ways. Is there one way to write a poem about the end of love? You can write a thousand poems and the next one will not be superfluous. Admitting that there are different representations in science is not at all a weakness – it is something of material and spiritual value, that builds a bridge between us and the people in the humanities.

There are more complicated molecules, such as thalidomide. In the 1960s a German chemical company put this molecule out in the market as a sleeping pill and in fact directed its marketing to pregnant women. In fact, the compound was teratogenic, the source of about 10,000 malformed births, mostly in Europe. The interesting thing is that the same molecule, which without doubt has caused incredible pain and suffering, has also a beneficial side. It is a proven therapeutic agent against a form of leprosy. It looks like a promising agent for the treatment of HIV infections and a number of other syndromes. One and the same molecule is both good and bad for people.

The human mind has a lot of difficulty with this idea, reflecting our own ambiguities on good and evil. Which leads me to the question: Are there good and evil molecules? No, there are no good and evil molecules, only good and evil people. Does the society have the right to restrict the production of a molecule even though the molecule is not good or evil by itself? You can argue with me, but I would say that indeed a society has the absolute right to restrict the production of a molecule.

Very often scientists avoid ethical discussions. In a caricature, they might say, "I am just making this molecule; it's not my responsibility to worry about what use you or someone else puts it to." If not I, who then? The world is made of such excuses, and less ethical people are waiting to use such scientists who refuse to think about the ethical consequences of what they do. I think it is a social responsibility of scientists to worry about the consequences of their actions, the molecules they make, and the techniques that they use, even if it is a danger to their jobs and to their own well-being.

Let's talk about the beauty in molecules – even simple-looking molecules, in the shape of Platonic solids – tetrahedral, cubes and even football shapes. These molecules are simply beautiful, beautifully simple, but devilishly hard to make. Except the last one. There is a remarkable irony in this, which serves as an inspiration to everyone working in science. Of all these molecules, by far the easiest to make is the one that was made last of all, and that's the football shaped one. What other things are waiting there to be made?

These molecules project their beauty, shine like a laser beam into our soul. When we see them we are happy. We are happier if we can make them. But wait a moment, simplicity is not all there is to beauty. There are more complicated molecules – take the oxygen carrier in our blood, hemoglobin. It looks like... worms doing a dance. Whatever this molecule is, with its 9,500 or so atoms, is in terms of a scale of simplicity and complexity, relative to the tetrahedron or a cube, light years away. This incredible molecule, with its four essential iron atoms, is certainly beautiful, on every account. But it has nothing to do with simplicity.

The beauty of hemoglobin resides in its function, of carrying oxygen to the lungs, and the way it is suited for it. I would like you to reflect on the fact that complexity is necessary to do things. A human body is not as simple as a liter of petrol. The human body runs lots of chemical reactions at the same time – breathing in, carrying the oxygen, getting the oxygen to the muscle cells, carrying the wastes away, there are at least 10,000 chemical reactions going on in us, and going on very quickly. You need complexity in order to do anything of value in this world. We have some trouble with this notion, probably because our mind, by itself a complex structure, somehow has evolved to favor simplicity, a weakness. This is something which politicians know well; their propaganda takes advantage of this weakness of ours.

Chemists can make structures that are simple, and they can also make molecules which are complex. It is an interesting kind of building we do – it's not at all like building a marble structure. Instead, we mix some chemicals and apply a source of energy, heat or light. Then we let go, and, incredibly, 10^{23} molecules colliding randomly inside a flask create what we want. With a little bit of design, and some luck.

Now there are structures that human beings build on a scale 12 orders of magnitude up from molecules. This is monumental architecture. What does it have to do with chemistry? Well, it is also building. It also takes money, takes talent, ergo human beings, all these things. Buildings and molecules are objects of human creation. What is interesting is that the structures that human beings have chosen to build in this world reflect some of the same questions of simplicity and complexity that are there in the world of molecules. The Taj Mahal of Agra, a high point of Mughal Architecture in India is clearly an expression of an aesthetic in which simplicity is valued. That is obvious in the dominant bilateral symmetry of the lovely structure. Though if you look at some details of the stone tiling and grillwork in the structure, you see tension, the juxtaposition of two different patterns. Symmetry sets repose, but interest is created by asymmetry. The towers of Chalukyan temples of the eighth and ninth centuries provide a good example of this.

I have come to the end of my second cross section of chemistry. As you've seen, this art, craft, business, and eventually science is firmly embedded in culture. Chemists have contributed their skills to the masterpieces of world art; art asks some of the same philosophical questions that chemistry does. Scientists take great risk in evading social responsibility for the magnificence of their creation. It is only by seeing both art and science as firmly embedded in our society, in our economy, in our culture, neither shirking ethical considerations, that we can move both forward. Together.