SCIENTIST AT WORK

Roald Hoffmann

Seeking Beauty in Atoms

By MALCOLM W. BROWNE

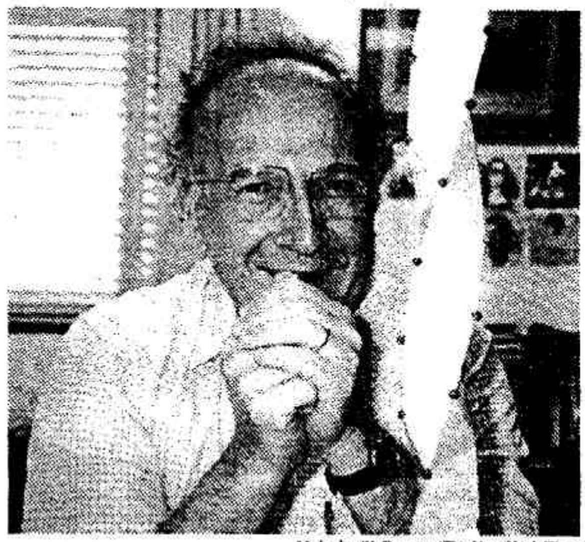
ITHACA, N.Y.

ROALD HOFFMANN — Nobel laureate, professor of chemistry at Cornell University and poet — glanced benignly at the stream of students passing his office window along a tranquil campus street. "I love chemistry," he remarked, "because it's sort of human in scale — infinitely complex, but always tangible, always real."

Although Dr. Hoffman's pursuits include such practical goals as finding a cheap substitute for one of the precious metals used in automobile catalytic converters, he is mainly interested in the beauty that he perceives underlying even mundane applications of chemistry. Dr. Hoffmann's students know that his conception of "beauty" in chemistry particularly refers to the subtle symmetries and asymmetries of electron "orbitals" in complex molecules. He was awarded the 1981 Nobel prize in chemistry for his idea that chemical transformations could be approximately predicted from these symmetries. His method gave chemists a powerful tool for predicting the pathways that chemical reactions may follow.

His life is driven by the urge to share this beauty with others, in the language of poetry as well as that of quantum mechanics. And so he he is also the author of a series of books of essays, criticism and poetry, the latest of which, "Chemistry Imagined," written with Vivian Torrence and published by Smithsonian Institution Press, draws scientific allusion into poetry in somewhat the way poets draw symbolic allusions from classical mythology.

The quest for beauty leads almost inevitably to interesting science, in his view. A molecule may be needed because it is useful to industry or essential to life, but the



Malcolm W. Browne/The New York Times

Dr. Roald Hoffmann, Nobel laureate in chemistry, uses theory, poetry and intuition in his laboratory.

best way to sketch it, Dr. Hoffmann says, may be to follow one's aesthetic sense rather than some mechanical recipe.

Palpable though chemical science may be, Dr. Hoffmann is not the kind of chemist who stains his fingers with laboratory reagents or cajoles recalcitrant salts into crystallizing from their solutions. He is a theorist

Continued on Page C10

Chemist Seeks Beauty in the Structure of Molecules and ir

Continued From Page C1

rand a poet, whose chemical intuition and personalized tool kit of mathematical tricks have pointed paths through many a knotty problem that had stumped experimentalists. Dr. Hoffmann's laboratory consists of his desk and his fountain pen, with which he produces graceful calligraphy as well as little pictures and diagrams much admired by other chemists, which symbolically describe the fruits of his theoretical research. He has barred all conventional laboratory paraphernalia — even computers — from his memento-cluttered office.

It is the awareness and appreciation of the aesthetic aspects of science rather than the mere toting up of numbers that leads to discovery, Dr. Hoffmann tells his graduate and postdoctoral students. In helping to impart this sense in them, he believes, he converts them into colleagues, fellow researchers as well as students.

At a recent symposium Dr. Hoffmann conducted for 10 of his fledgling scientists, the deceptively simple assignment had been to bring anything to the meeting that seemed interesting or beautiful.

At the end of two hours, the students, including one Russian, one Mexican and two Chinese, had analyzed, discussed and pondered enough material to launch a couple of doctoral dissertations, despite the group's steady stream of wisecracks over pizza and soft drinks.

"You can see why it is impossible for me to distinguish between teaching and research, much though the accountants would like me to do so," Dr. Hoffmann said later. "Science is a bridge between teaching and discovery, and my life has been spent building bridges."

Dr. Hoffman was born Roald Safran on July 18, 1937, in Zloczow, a town in the part of Poland that was later absorbed by the Soviet Union. After the German invasion in 1939 he and his parents, Hillel and Clara Safran, were sent to a labor camp as part of the Nazi roundup of Jews. Roald and his mother escaped, but Mr. Safran remained in the camp to help organize a breakout. The plan was betrayed, Mr. Safran was killed, and his wife and son remained hidden in the attic of a schoolhouse for the rest of the war.

Having survived the war, mother and son emigrated to the United States in 1949. His mother remarried and the boy took his stepfather's surname — Hoffmann. The name Roald had been bestowed on him in honor of Roald Amundsen, the great Norwegian polar explorer.

Young Roald got such good grades in science that he was accepted at Stuyvesant High School — one of New York City's preeminent science schools. "The concentration of intellect was really higher at Stuyvesant than anywhere else in my experience, including Columbia College and Harvard University graduate school," he recalls.

His academic experience at Columbia nearly diverted him from a career in science.

"At the time, Columbia's chemistry department was not as inspiring as the humanities departments. Mark Van Doren taught me poetry, I studied Japanese literature and I almost switched my major to art history.

"Like many middle-class American Jewish parents, mine wanted me to be a doctor, so I majored in premed, and the premed courses included chemistry. The chemistry fascinated me, and eventually I found the strength to declare that I would not become a doctor but would become a chemist," he said.

But he soon discovered that he was not cut out to be a laboratory chemist. "In graduate school, one time, I was supposed to synthesize a compound — a polyphenyl porphyrin — using a sealed pressure vessel to contain the reaction. I didn't seal it properly, and the thing blew up, demolishing a fume hood and smearing gunk all over a brand new laboratory. That marked

'Mark Van Doren taught me poetry, I studied Japanese literature . . .'

the end of my career as a synthesis chemist," he said.

The work for which Dr. Hoffmann is best known has to do with orbitals — the quantum-mechanical "wave functions" of electrons that surround the nuclei of atoms and which are responsible for all chemical interactions. A wave function of an electron is the probability of its being in any possible place. Wave functions can be positive or negative, they interact with each other, and they provide the glue that links atoms to form molecules.

In a molecule, the wave functions of the electrons of individual atoms interact with those of other atoms in patterns more complicated than those of a Rubik's Cube. In matching up orbitals to see if some desired pattern (that is, some hypothesized molecular structure) is possible, vast numbers of quantum-mechanical calculations are ordinarily needed. But by extending and expanding on a method devised in the 1930's by Erich Hückel, a German chemical theorist, Dr. Hoffmann found a way to make what he calls "very poor quality but very useful" quantum calculations, which yield approximate predictions of how chemical interactions will procede. These predictions sometimes turn out to be wrong, Dr. Hoffmann says, which is why the special insights of an experienced chemist are needed to distinguish probably correct results from implausible ones.

It is this kind of calculation that Dr. Hoffmann (and legions of other chemists) use today in attacking new reaction and synthesis problems. Sometimes Dr. Hoffmann and his students provide theoretical blueprints for creating interesting but useless molecules. At other times, the blueprints solve such highly practical puzzles as how the various components of electronic chips form chemical bonds with each other.

"It's difficult to explain our work to people who don't know quantum mechanics," he said. "But I sometimes use an analogy of a hostess seating people around a table who must all be matched up by sex or social position or something. You must have certain numbers of people and certain arrangements to make the seating come out right. It's somewhat the same with molecular orbitals."

This kind of research involves a great deal of fundamental physics, but Dr. Hoffmann vehemently denies that he is a physicist.

"When I try to explain chemistry to outsiders," he said, "I have three main audiences: the person in the street, fellow academics in the humanities and physicists. All three audiences are equally ignorant of chemistry, but the most difficult audiences are the physicists, because they think they understand, but they don't."

He added: "Chemists don't have any Holy Grail, like the quest by particle physicists for the top quark or Higgs boson. Our goals are small
but numerous, on the scale of
human condition itself."

A great shortcoming of theoret
physics, Dr. Hoffmann believes,
that physicists tend to be reduct
ists: they believe that everythin
nature can be reduced to a few sim
principles and particles. "Neither
ture nor life works that way in re
ty," he said. "Complexity, not s
plicity, is the essence of life. Take
molecules — say, dodecahedran
nice, simple, soccer-ball-shaped
ecule, which has no use, and hemo
bin, an incredibly convoluted, c
plex molecule. For me, the hemo
bin is the more beautiful because
and not despite, its complexity.
complex form is essential for d
the complex things it has to
Hemoglobin is the compound in
blood cells that chemically captu
oxygen from the airways and tr
ports it to the body's tissues.

Despite his frequent criticism
certain branches of physics, Dr. H
mann insists that he has no gen
bias against the field; his own dau
ter, Ingrid Hoffmann, recently
ceived a Ph.D. in solid-state phy
and is now doing research on Gre
land's ice cap.

But Dr. Hoffmann chides so
physicists for their concentration
the ultra-large — the entire unive
— and the ultra-small, the fundam
tal particles making up atoms.

"Chemistry is an intermediate
ence between the extremes of s
more in consonance with the hum
scale of things," he said. "We ch
ists are down-to-earth people,
are not so troubled with the my
cism that sometimes creeps
physics. For example, I use quant
mechanics constantly, just as an
gineer uses cement. But I don't a
nize over its paradoxes the way so
physicists do."

Dr. Hoffmann likes to take d
from other experimental laborato