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 about 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, Robert 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 nonintuitive 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 world—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. 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 show 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 psychologist Jerome Bruner 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 Bruner's phrase.

Storytelling seems to be ingrained in our psyche. I would claim that with our gift of spoken

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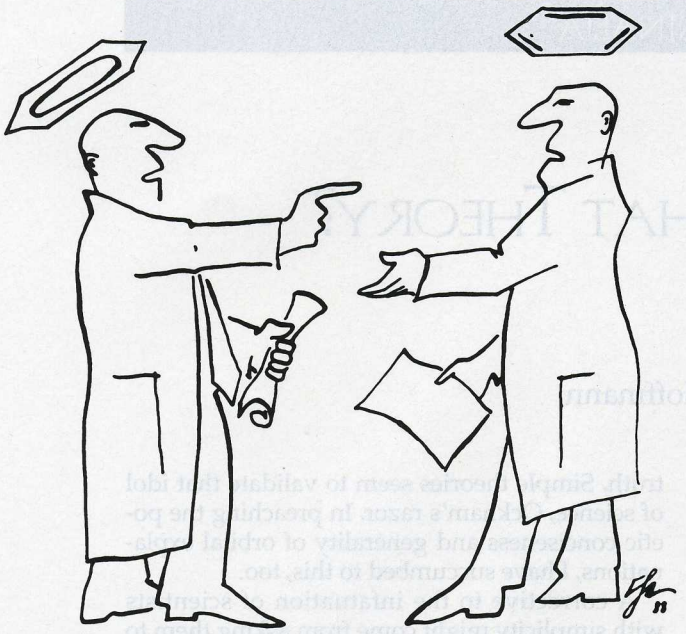

Cartoon by Constance Heller, originally published in 1988 (*Angewandte Chemie* 100:1657).

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 towards 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 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 Erector set, 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 there is in person A advancing a view of how things work, which is tested by B, used by C to motivate making a molecule that tests the limits of the theory, which leads to D (not C) finding that molecule to be superconducting or an antitumor agent, whereupon a horde of graduate students of E or F are put to making slight modifications! People need reasons for doing things. Theories provide them, surely to test the theories (with greater delight if proved wrong), but also just to have a reason for making the next molecule down the line. Theories that provoke experiment are really valued by a community that in every science, even physics, is primarily experimental.

A "corollary" of the significance of productivity is that theories that are fundamentally untenable or ill-defined can still be immensely productive. So was phlogiston in its day, so in chemistry was

the idea of resonance energies, calculated in a Hückel model. People made tremendous efforts to make molecules that would never have been made (and found much fascinating chemistry in the process) on the basis of "resonance energies" that had little connection to stability, thermodynamic or kinetic. Did it matter that Columbus miscalculated in his "research proposal" how far the Indies were?

As Jerry Berson has written, "A lot of science consists of permanent experimental facts established in tests of temporary theories."

Frameworks for Understanding

Stephen G. Brush has recently studied a range of fields and discoveries, to see what role predictions play in the acceptance of theories. Here's what he has to say about the new quantum mechanics: "Novel predictions played essentially no role in the acceptance of the most important physical theory of the 20th century, quantum mechanics. Physicists quickly accepted that theory because it provided a coherent deductive account of a large body of known empirical facts...." Many theories predict relatively little (quantum mechanics actually did eventually) yet are accepted because they carry tremendous explanatory power. They do so by classification, providing a framework (for the mind) for ordering an immense amount of observation. This is what I think 20th century theories of acidity and basicity in chemistry (à la Lewis or Brønsted) do. Alternatively, the understanding provided is one of mechanism—this is the strength of the theory of evolution.

It is best to distinguish the concepts of theory, explanation and understanding. Or to try to do so, for they resist differentiation. Evelyn Fox Keller, who in her brilliant recent book, *Making Sense of Life*, has many instructive tales of theory acceptance, says this of explanation:

> A description or a phenomenon counts as an explanation ... if and only if it meets the needs of an individual or a community. The challenge, therefore, is to understand the needs that different kinds of explanations meet. Needs do of course vary, and inevitably so: they vary not only with the state of the science at a particular time, with local technological, social, and economic opportunities, but also with larger cultural preoccupations.

As Bas van Fraassen has incisively argued, any explanation is an answer. If we accept that, the nature of the question becomes of essence, and so does our reception of the answer. Both (the reconstructed question of "why?" and our response) are context-dependent and subjective. Understanding, van Fraassen says, "consists in being in a position to explain." And so is equally subjective in a pragmatic universe.

Incidentally, explanations are almost always stories. Indeed, moralistic and deterministic stories. For to be satisfying they don't just say A→B→C→D, but A→B→C→D *because* of such and such propensities of A, B and C. The implicit strong conviction of causality, justified by seemingly irrefutable reason, may be dangerously intoxicating. This is one reason why I wouldn't like scientists and engineers to run this world.

The acceptance of theories depends as much on the psychology of human beings as on the content of the theories. It is human beings who decide, individually and as a community, whether a theory indeed has explanatory power or provides understanding. This is why seemingly "extrascientific" factors such as productivity, portability, storytelling power and aesthetics matter. Sometimes it takes a long time (witness continental drift), but often the acceptance is immediate and intuitive—it fits. Like a nice sweater.

'Tis a Gift

There is something else, even more fundamentally psychological, at work. Every society uses gifts, as altruistic offerings but more importantly as a way of mediating social interactions. In science the gift is both transparent and central. Pure science is as close to a gift economy as we have, as Jeffrey Kovac has argued. Every article in our open literature is a gift to all of us. Every analytical method, every instrument. It's desired that the gift be beautiful (simple gifts are, but also those that bring us a good story with them), to be sure. But that the offering be useful (portable, productive) endows it with special value. The giver will be remembered, every moment, by the one who received the gift.

The purpose of theory, Berson writes, is "to bring order, clarity, and predictability to a small corner of the world." That suffices. A theory is then a special gift, a gift for the mind in a society (of science, not the world) where thought and understanding are preeminent. A gift from one human being to another, to us all.

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