

Marginalia

Nearly Circular Reasoning

Roald Hoffmann

Scientific argument is supposed to be logical. But do scientists study logic? Probably not. Were they asked about the advisability of learning formal or applied logic, most would likely say, "Logic, as studied by philosophers, is just a systematization or description of what we, as scientists, do naturally. So we don't need to study it."

The chain of reasoning that I've ascribed here to a straw-man scientist is, on analysis, full of the fallacies described by Aristotle in *Sophistical Refutations* (*De sophisticis elenchis*) more than 2,300 years ago. The argument suffers from circular reasoning, the fallacy of false cause, the argument *ad populum* (the *populus* here being scientists, as opposed to philosophers), and more (1). But actually I do not want to berate here the logically unsophisticated scientist (myself), nor to urge that scientists need study philosophy. Rather, I'd like to examine the curious role of logic in science. Good logical thinking is absolutely necessary to both everyday and revolutionary science. But I will argue that at the same time, reasoning in all science, paradigmatic or ground-breaking, on close scrutiny often turns out to be in part illogical. There is nothing new in this—we see readily the fallacies in the work of others, especially when they disagree with us, don't we? I will try to make a case, however, that there may be a real advantage implicit in occasionally faulty reasoning, especially a mode which I will call nearly circular reasoning.

Science is a curious mixture of the real and the ideal, the material and the spiritual, held together by discourse or argument. The latter is sometimes mathematical, but more often it transpires in the words of some language. The real is the material, say, a vial of a chemical, or its measured spectrum, the relative amount of light a solution of that chemical absorbs. The ideal may be a proposal on the mechanism of formation of the molecule, or a theory that interprets that spectrum as necessarily indicating the molecule contains a carbon-hydrogen bond. The discourse consists of the exposition of several arguments, several alternative models explaining the observable, and a choice between them. Try to imagine a scientific article or a seminar without the glue of words or argument!

The use of language, an absolute necessity in scientific discourse, is one source of possible circularity; the nature of argument is another. A cursory tracing of chains of definitions in any dictionary reveals how quickly such chains become circular. Yet we easily use language to explain and communicate. As Klever says, "Natural language is a complex network in which circular argumentation is not only unavoidable, but even the only means of explication" (2).

Argument has perforce a psychological and rhetorical component—it is an attempt to convince, first oneself, then others, of the validity of a certain conclusion. The dialogue may be an inner one, shaping ideas or prompting one to do the next experiment. It may be an

outer one, with imagined audiences as one writes a paper, with real ones at a scientific conference. It is in these rhetorical settings that the natural argument of scientists becomes quasicyclic.

Yet, by being connected on one hand to the reality of substances and measurements, on the other hand tied to the inner psychological forces that move us, that possibly illogical argument advances science.

Productive argument in science is mostly about new things. Recently, high-temperature superconductors of two kinds were discovered, $\text{La}_{1.85}\text{Ba}_{0.15}\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{\sim 7}$. If one takes the oxidation states (a tremendously useful fiction) of lanthanum and yttrium as 3+, oxygen as 2-, and barium as 2+, then in both cases one comes to the conclusion that one is working with copper atoms in oxidation states between 3+ and 2+. Perhaps some coppers are 3+, some are 2+, just enough to make that balance right. One can begin to build theories which link the extraordinary conductivity to some precarious balance of the energetics of copper ions in different oxidation states (3).

Meanwhile, several groups have recently come up with evidence, from a measurement involving x-ray spectroscopy, that in these ceramics there is another type of oxygen ion, in addition to the normal "2-" one (4). If it's there, it's important, because if you follow through the charge balance, the coppers don't have to bear so much positive charge if some of the oxygens are O^- instead of O^{2-} . In fact, instead of Cu^{3+} and Cu^{2+} , the discussion shifts to Cu^{2+} and Cu^{1+} . Which, for various reasons, would make chemists happier.

Since oxidation states are a convenient fiction, we mustn't take O^{2-} and O^- too seriously (5). A realization of "O-" would be peroxide ions: O_2^{2-} , diatomic entities. There is an argument building as to whether, in these superconductors, some of the oxygen atoms might have moved off their idealized lattice sites, where they are too far apart to bond, to form peroxide ions. The argument will soon draw in the structural chemists and physicists who determined the positions of the atoms in these substances. Because there is some disorder in these molecules as a result of the oxygen nonstoichiometry, these structures—the best that can be done—are not as accurately known as other stoichiometric solids. Whatever the crystallographers did, and I repeat that they did it very well, and in nine laboratories (or is it seventeen?), it was assumed that the oxygens always sit at certain lattice sites, with no O_2^{2-} or peroxide species present. Well, they're going to go back and think about it.

Some day, there will be definitive proof of the absence or presence of O_2^{2-} units. But then the problem will be solved, dull, and uninteresting. Today there is no proof, the problem is actual—there are just hints, the merest trace of a shoulder in a complex spectrum, less than that. Right now intuition, a jump of the imagination, a nondeductive argument, the following of a hunch can matter. And the published literature, still more the oral presentations at seminars and meetings, and still much more the informal opinions voiced in research

Roald Hoffmann is professor of chemistry at Cornell University.

group meetings, are full of suppressed or explicit opinions and categorical statements that such-and-such a measurement or theory is nonsense. There is rash judgment, there may be prejudice, there certainly is a lot of disagreement. In the debate that ensues, logic is likely to play a significant role. Nevertheless, because it is a debate, and human beings rather than machines are

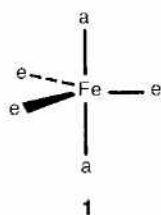
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debating, it is likely that the full spectrum of rhetorical tricks and fallacies that Aristotle saw so clearly will be involved—nearly as much in this discussion as in the forthcoming presidential campaign.

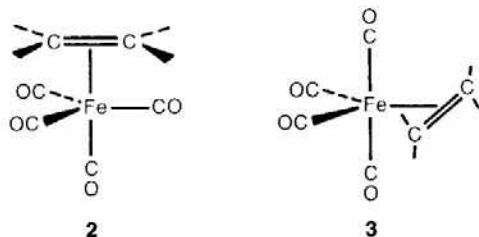
But what people will do to win an argument or convince others is really not what I want to address. I want to examine some of the ways in which fallacies or illogical thought may be useful in science.

Constructing an explanation or rationalization, then claiming it as a prediction, validating the theory so constructed, seems patently illogical. But I will claim that the process has definite value. Since I get into mighty trouble if I use the work of living or recently deceased colleagues, I'm left with illustrations from my own work or that of people long dead.

Iron-tetracarbonyl-ethylene, $\text{Fe}(\text{CO})_4(\text{C}_2\text{H}_4)$, is an interesting molecule, known for over twenty years, and quite typical of modern organometallic compounds. Its shape can be described as an iron-centered trigonal bipyramid, or two tetrahedra sharing a face, with an iron in the middle. Structure 1 illustrates the geometry; in it there are distinct axial (a) and equatorial (e) sites.

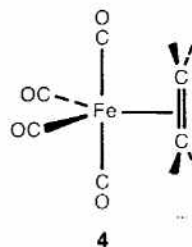


To a chemist the obvious question is whether the ethylene occupies an axial site, as shown in structure 2, or an equatorial site, as in 3. The experimental answer, coming from x-ray crystallography, is that shown in structure 3, ethylene equatorial (6).



With that established, a further question may be posed: is the carbon-carbon bond of the ethylene oriented in the

equatorial plane (as in 3), or perpendicular to that plane (i.e., parallel to the vertical axis, as shown in structure 4), or somewhere in between?



When my co-workers and I constructed a theory of the geometry of this molecule and other organometallic compounds about ten years ago we knew of several experimentally determined structures, all of which showed the ethylene in an orientation near to structure 3. In our explanation we constructed 2, 3, and 4 from the orbitals of an $\text{Fe}(\text{CO})_4$ fragment and ethylene, and showed that the favored arrangement was ethylene equatorial and that there was a strong preference for the specific geometry illustrated in 3.

When we found our argument for the observed geometry of structure 3, we didn't say that we merely "rationalized" the known preference. Neither did we dare say that we "predicted" it, for that would clearly have been too much, a number of experimental structures already being known at the time. In typically ambiguous (or sloppy) language we said that a certain quantum-mechanical interaction "will cause a marked preference for the coordinated ethylene to be in the equatorial plane." Note the subtle appeal to strong causality, a hint that this is the way things must be.

Actually, I think that our argument, whose details are quantum-mechanical, was not a case of circular reasoning. But in the explanation we were admittedly reaching for the status of a prediction. Why? Because, of course, a true explanation must have consequences of a predictive nature. The subtle conversion of a rationalization into a prediction was probably even stronger in our minds than we allowed ourselves to commit to paper. Was this bad?

Not really, I think, and here I will leave my own failing and generalize that much of this, very much, goes on in the work of others. What we gained as a result of that bit of almost circular reasoning is confidence. We were not engaged in a mathematical proof, we were doing chemical theory. Theoretical chemistry, at the level we were practicing it, is happy if it is right 85% of the time on the geometry of a molecule. It is soft theory. So is most theory in science, although the ideology of science tends to single out hard theories—those capable of being disproved by a single experiment—as being emblematic of all theory (7). This is a romantic fantasy, and science, not only chemistry, would have gotten nowhere if it had waited for such strong theories. The reasoning used by Bednorz and Müller in their discovery of the high-temperature superconductors is a good example of this (8). They came to their remarkable discovery by a wonderful, chemical process of hints, analogies, facts, and intuition.

When one is in the act of building a theory, a framework for understanding, one needs all the psycho-

