

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

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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

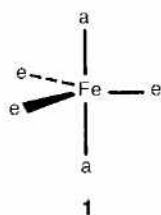
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debating, it is likely that the full spectrum of rhetorical tricks and fallacies that Aristotle saw so clearly will be involved—nearly as much in this discussion as in the forthcoming presidential campaign.

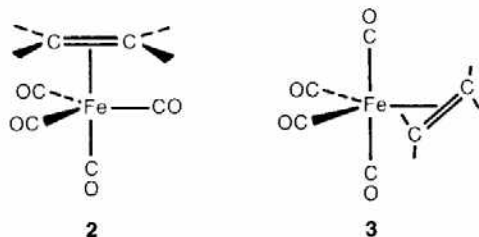
But what people will do to win an argument or convince others is really not what I want to address. I want to examine some of the ways in which fallacies or illogical thought may be useful in science.

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.

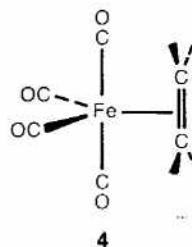


To a chemist the obvious question is whether the ethylene occupies an axial site, as shown in structure 2, or an equatorial site, as in 3. The experimental answer, coming from x-ray crystallography, is that shown in structure 3, ethylene equatorial (6).



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.

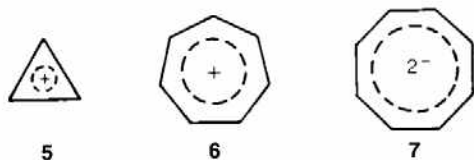
When one is in the act of building a theory, a framework for understanding, one needs all the psycho-

logical support one can get. When it's all done, it's stuff for textbooks on the scientific method or for sanitized memoirs. But when it's being done, one grasps at straws. One wants a theory to "work." And so when it does work one is happy, encouraged to put in the terrible labor that is often involved in pushing through to the next calculation, the next prediction.

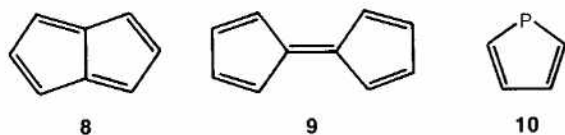
There is another imperative for circularity, inherent in the natural interplay of theory and experiment. One has curious observations, begging for explanation. So one explains them, constructing a trial model, a theory. To see if it works one compares the theory's results with experiment. Note the forward and reverse motion that shapes the circle. If the theory doesn't quite explain all the anomalous observations, then one thinks harder, refines the model. The circle tightens. The way out is a prediction that is new, unexpected.

Fallacious reasoning can play a useful role in experiment as well as in theory. One needs a reason for doing something—it doesn't matter what the reason is. If this is an existentialist argument, so be it. A clever person, with a will to experiment and the proper tools at his or her command, the most important tool being an open and inquisitive mind, can find interesting science in a study undertaken, in retrospect, for the weirdest reason.

In the late 1940s there was a remarkable validation of Hückel's rules for the stability of conjugated electron systems (9). Molecules predicted to have large resonance energies were suddenly being made in the laboratory: the cyclopropenyl cation shown in structure 5, cycloheptatrienyl cation in structure 6, and cyclooctatetraenyl dianion, structure 7.



These aromatic rings conformed readily to the far-reaching $4n + 2$ rule (the number of π -electrons in these molecules). At the same time it became easy to calculate a simple quantity called the "delocalization energy," which was found to be high for these molecules. It was also high for other molecules that had not yet been made, such as pentalene (structure 8), fulvalene (structure 9), and many heterocycles, of the type shown in structure 10. Organic chemists around the world were spurred on to make these molecules.



But the theoretical reasoning behind these extensions of Hückel's method was weak; the concept of a resonance energy, simplistically defined as it was then, invalid. The molecules that were synthesized were often kinetically unstable. Was this a wasted effort? Should the experimentalists have waited for a better theory? They would be waiting still. Fascinating molecules, some of pharmacological utility and some leading to novel con-

ducting systems, were made, all chasing a wrong theory.

There's more to it than doing the right thing for the wrong reason (10). Let's take a typical planned organic synthesis of some complex natural product. In a sequence of 20 to 30 steps, actually hundreds of physical operations, a complicated molecular architecture is constructed. The process is all the more incredible for being a hands-off kind of building. The reagents in each step are mixed, energy is put in in some way, and, voilà, 10^{20} molecules do what we would like them to have done, while the entropy of the universe increases. Or so it appears in the published paper.

But along the way things were different. The reaction steps remain marvelous. In proceeding through

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each step the designers and executors of the synthesis certainly begin with a plan. A bond must be formed, and carbon A should attack carbon B just on this side of a plane, and not on the other. The professor remembers a paper in which such a reaction took place under certain conditions. He advises a graduate student to try it (this is called "precedent," but in the absence of further reasoning it may shade over into the fallacy of appealing *ad antiquam*. Antiquity in science is usually two years old.). It almost never works on the first try, and often doesn't on the tenth try as well. The graduate student, unwilling to tell the professor that the latter's magnificent plan has failed, asks a postdoctoral fellow working in the same group if he has seen any other way to effect the reaction. The postdoc suggests that perhaps a method he saw in an obscure paper might work. The reasoning proceeds often by crudest analogy, or by primitive ideas that no one wants to admit to in print. This suggestion fails on the first try, too, but then the graduate student changes the order of mixing the reagents, and the synthesis works! He then optimizes the yield, because he knows that his professor knows that the community views a high yield as a sign of elegance and control. There is a happy ending in this for all: the student, the professor, and the whole field of chemistry admiring the ingenious synthesis. How clever of them to apply that reaction (the one that worked) in the most difficult step in the synthesis!

Curious—the true ingenuity and originality that was exhibited in real life, in exploiting the magnificent aleatory process that is much of science, is masked because of some hidden insecurities as to the "illogical" way in which key choices were made.

One might argue against my thesis of a real role for fallacy by pointing out that science could not advance if all arguments were circular or suffering from other failures of logic. I agree that much of paradigmatic science follows logical straight lines. The failures of logic do not impede the progress of science but seem to provide a mechanism for including random deviation as a productive shock setting the system off the beaten track. The awesome motive force of individual psycho-

logical conviction then propels one to true innovation. Science as a whole progresses because it is not derailed by isolated failures of logic. But in analyses of the way science works one always chooses simplified cases, unrealistic ones. In these one can only see that circular reasoning is bad. One can't conceive of nearly circular reasoning.

Let me give an analogy. It has been shown that one cannot have a true phase transition, a cooperative phenomenon in one dimension, but can have one in two or three (11). In one dimension a chance mistake in spin alignment ruins everything—there is no way of communicating information, some favored alignment, past that mistake. In more dimensions than one the linkage is essentially tighter; there is a way, many ways for information to pass “around” the mistake. Well, I think science is like that, an intellectual enterprise in a space of immense dimensionality—at least the product of the number of practitioners and the number of objects of their study. Looking at a piece of circular reasoning isolated out of the context of thousands of people reading of the work of others, using it, testing experiments, is like trivializing many dimensions to one.

The closed circle is nonproductive, even if it served Kekulé. My metaphor is the nearly closed circle. One end moves, thinks it is free. It doesn't know how near it is to forming a true circle, it knows it should avoid it, yet the forces that shape its motions keep pressing it near its origin, onto itself. In the space between the end and the beginning, in that little space, it uses the tension of resisting junction to carve out marvels, a universe (12).

References

1. For a hilarious introduction to fallacies see M. Pirie, 1985, *The Book of the Fallacy*, Routledge and Kegan Paul.
2. The reader's attention is directed to a remarkable article (in Dutch, with English summary) addressing many of the points made in my column. It is by W. N. A. Klever, 1982, *Tijdschrift v. filosofie*, 44:603. The article, entitled “Circular Argumentation,” was brought to my attention by Sven Ove Hansson; I thank Marja Zonneville for her translation. For a perceptive discussion of related problems, see E. W. Beth and J. Piaget, 1961, *Epistémologie mathématique et psychologie*, Presses Universitaires de France, pp. 294–99.
3. See, for instance, A. W. Sleight, 1987, in *Chemistry of High Temperature Superconductors*, ed. D. L. Nelson, M. S. Whittingham, and T. F. George, p. 2. American Chemical Society, Symposium Series 351.
4. Some leading references, as they say, are: D. D. Sarma and C. N. R. Rao. 1987. *J. Phys. C: Solid State Phys.* 20:L659. R. A. de Groot, H. Gutfreund, and M. Weger. 1987. *Solid State Comm.* 63:451. B. Dauth, T. Kachel, P. Sen, K. Fischer, and M. Campagna. 1987. *Z. Phys. B.—Cond. Matter* 68:407.
5. See the discussion in ref. 3. Attitudes toward formal oxidation states are another illustration of the differences in language between chemistry and physics that I discussed in *Am. Sci.* 75:619 (1987).
6. See ref. 17 in T. A. Albright, R. Hoffmann, J. C. Thibeault, and D. L. Thorn, 1979, *J. Am. Chem. Soc.* 101:3801.
7. The characterization of theories here as soft or hard connects up to the idea of strong inference, as described by J. R. Platt, 1964, *Science* 146:347. Obviously I don't agree with this paper on many matters.
8. K. A. Müller and J. G. Bednorz. 1987. *Science* 237:1133.
9. See, for instance, chapter 2 in J. March, 1985, *Advanced Organic Chemistry*, 3d ed., Wiley.
10. T. S. Eliot. 1935. *Murder in the Cathedral*, p. 44. Harcourt Brace Jovanovich. For an apposite citation, see J. Meinwald, A. Eckell, and K. L. Erickson, 1965, *J. Am. Chem. Soc.* 87:3532.
11. L. van Hove. 1950. *Physica* 16:137. R. Peierls. 1936. *Cambridge Phil. Soc.* 32:477. R. B. Griffiths. 1964. *Phys. Rev. A* 136:437.
12. In the writing of this paper I benefited from discussions with Sven Ove Hansson, Barry Carpenter, Paul Houston, and Ben Widom.



“Now that we've come up with a sweetener 650 times sweeter than sugar, we're working on a sourer 475 times sourer than a lemon.”