

# ON THE RELEVANCE OF REPETITION, RECURRENCE, AND REITERATION

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## Abstract

Recently, some philosophers have claimed that widely accepted notions of causality are inadequate for dealing with human action. Related considerations also apply to much simpler systems that chemists encounter. In order for a chemical entity (molecule, dissipative structure, etc.) to exert significant influence, that entity must possess internal coherence — and also must maintain its integrity during interactions with other entities. A balance of opposing internal tendencies characterizes every chemical entity. Each inevitably has internal flexibility — and that flexibility is necessarily limited. Every chemical entity executes continuous oscillations. Particular detailed states of the components of the system recur periodically. A *closed set* of interactions specifies the pattern of repetitive alterations that is characteristic of each entity. That closure of relationships is the explanation, or reason, or cause, of the stability of the entity. The same closure regulates the efficient causality from which the coherence itself originates and also determines whatever influences that entity may exert on others. Any account of chemical phenomena that ignores these (formal) aspects of causality is incomplete.

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**I**

John Maynard Keynes once observed (Keynes, 1936): "Practical men, who believe themselves to be quite exempt from any intellectual influences, are usually the slaves of some defunct economist." Keynes, an economist himself, was talking to and about businessmen, but the point also applies to physical scientists. All of us, even chemists, are deeply influenced by doctrines, decisions, and preferences of long-dead philosophers — whether or not we are conscious of being so shaped.

This paper concerns *causes*, from both philosophical and chemical points of view. I first summarize recent claims of Alicia Juarrero (1999) and Ernan McMullin (1999) concerning a change in the notion of causality that, they assert, occurred in the

late Renaissance. Then, I use examples from contemporary science to support the suggestion that these two philosophers make that current concepts of causality are seriously deficient. The first topic scientific topic will be the connection between chemical bonding and molecular vibration. Then two examples (one from the origin of the elements and one from industrial chemistry) will be described — as fairly practical illustrations of the fact that the details of how coherences are held together is critical to their functioning. The next section will summarize recent developments in statistical mechanics that indicate that this result is fundamental rather than merely practical. Another section of the paper outlines how combinations of processes (as well as collections of particles) can yield long-lived coherences that have specific effects on the rest of the world. The last section of the paper points out that in all the examples cited, details of interaction of components control which potentially efficient interactions are effective, indicating that received notions of causality need to be supplemented by greater emphasis on the importance of structure (*née formal cause*).

A usual starting place for philosophic consideration of causality is the section of Aristotle's *Physics*<sup>1</sup> (Barnes, editor, 1984, page 33.) that introduces his four types of causes — material, formal, efficient, and final. McMullin suggests that readers should pay careful attention to the preamble to this section. That introductory portion shows that what Aristotle himself meant by cause is different in important ways from what we now generally understand by that term, influenced as we are by more recent

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1. *Book II* (194b, 17 B 195a, 3).

developments in science and in philosophy. The introduction to Aristotle's first discussion of the four causes reads:

Knowledge is the object of our inquiry, and men do not think they know a thing until they have grasped the '>why' of it (which is to grasp its primary cause). So clearly we too must do this as regards both coming to be and passing away and every kind of natural change, in order that knowing their principles, we may try to refer to those principles each of our problems.

McMullin and Juarrero both claim that the notion of cause underwent subtle but significant change after the triumph of Gallilean-Newtonian mechanics in the seventeenth and eighteenth centuries. With the success of physics in rationalizing both Renaissance astronomy and everyday mechanical technology, impact of impenetrable corpuscles in collision became the paradigmatic sort of cause. *Efficient* causality assumed pride of place, and largely took over the name of cause. All the other kinds of influences that previously had been designated as causes were relegated to subordinate status. Significant causal interactions came to be considered to resemble events on billiard tables, where a precisely determined impact yielded exactly predictable results. That there has been a major change in the idea of cause can be seen in the difference between the synonyms given by Aristotle's modern editor for the Greek word that is normally translated cause and a contemporary dictionary definition of how the word

cause is used in present-day English. Jonathan Barnes, Aristotle's editor, glosses<sup>2</sup> the Greek word *aitia*, (*aition*) as explanation or reason. *The Shorter Oxford English Dictionary* gives four meanings for the word cause. The first three<sup>3</sup> are: 1) that which produces an effect, 2) motive, 3) lawsuit. That which produces an effect means *efficient* cause. The Greek term translatable as 'reason' had a much wider scope — a range that is not spanned by any of the meanings given for the contemporary usage of the word cause. We are all influenced by the conceptual shifts that accompanied the rise of modern science. Change in the notion of cause is one instance of this influence, whether or not we may approve this change.

In its day, the move to restrict the notion of cause to efficient factors may well have been beneficial. By the sixteenth century, the Scholastic philosophic system, dominant since the medieval period, had extended itself beyond the effective support of its foundations. Scholastic philosophy was no longer capable of dealing with the problems that interested scientific and cultural leaders of the day. The notion that causality was exclusively efficient helped purge philosophy of unfortunate excesses.

But as Alfred North Whitehead (1967, page 59) observed: .."if men cannot live on bread alone, still less can they do so on disinfectants". Juarrero argues persuasively

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2. Barnes, editor (1984). *Op. cit.* page 2472.

3. The fourth meaning has to do with cause as the unifying aim of an ideology or movement, a quite different usage.

that the restricted notion of causality adopted with the rise of modern science is an impoverished one — a concept that is totally inadequate for philosophical analysis of human action. Billiard-ball causality is not much use in telling "the difference between a wink and a blink." But we need not get into the complexities of human action in order to recognize the problem that Juarrero identifies; it is apparent even in such a relatively uncomplicated field as chemistry.

## II

The first scientific example that we consider is bonding within chemical molecules. At the beginning of the twentieth century, relatively little was known about how atoms were held together in compounds. By the end of that century, the question of chemical bonding was, to all intents and purposes, closed — a quite complete and highly satisfactory scientific account of combination of atoms into molecules (and molecular ions) had been achieved.

What specific molecule should we consider to illustrate this discussion? We follow venerable tradition and examine the hydrogen molecule —  $H_2$ , now called *dihydrogen*. Every educated chemist can describe how the internal potential energy of dihydrogen varies as with change in the distance between the two hydrogen nuclei (protons) that account for the bulk of the mass of the molecule. At low values of proton-proton distance, the energy is positive — that is, repulsive. If the two positively charged protons happen to be close to each other, there will be a strong repulsion of like charges — and a high tendency for the two nuclei to move apart. But if the two hydrogen nuclei

(protons) are widely separated, potential energy is negative, since the two positive hydrogen nuclei are attracted to the pair of negatively charged electrons that they share. That attraction decreases (potential energy approaches zero) as the distance between the protons increases. At intermediate proton-proton distances, potential energy becomes quite negative — the two positive protons and two negative electrons are strongly attracted to each other. If the two protons are either further apart or closer together than a certain specific distance (called *the equilibrium inter-nuclear distance*) the components will tend to move towards that spacing. The minimum value of potential energy (reached at the equilibrium inter-nuclear distance) is numerically equal to the amount of energy that would be needed to tear the molecule apart — designated *the bond energy*. Successive advances in theory have enabled chemists accurately to compute energy-distance relationships for the dihydrogen molecule *a priori* (from basic principles of electrostatics and quantum mechanics). It seems fair to say that, for the dihydrogen molecule, 'the why' of the variation of potential energy with inter-nuclear distance is as well understood as is any other important feature of human culture.

At all finite temperatures, each dihydrogen molecule vibrates about the proton-proton distance that corresponds to the potential energy minimum, repeatedly cycling between stretched arrangements and compressed configurations, passing through a large<sup>4</sup> set of specific intermediate arrangements on the way. At any temperature above absolute zero on the Kelvin scale, the molecule vibrates continuously, without pause or

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4. Strictly speaking, this is an infinite set.

interruption. As temperature increases, the vibration gets more energetic — faster and with greater amplitude<sup>5</sup>. When a particular dihydrogen molecule collides with another one — or with some surface — energy may be transferred, but vibration does not cease. Radiant energy (such as ultraviolet, infrared, or visible, light) can sometimes be absorbed by the dihydrogen molecule and converted into internal vibrational energy. Because the bond energy of dihydrogen is substantial, absorption of highly energetic ultraviolet light would be required to split the dihydrogen molecule into its constituent atoms.

The flexible vibratory motion — reiteration, recursion, repetition, of a set of molecular configurations — allows the collection of two protons and two electrons (with assorted vector particles) that comprise the dihydrogen molecule to *act as one unit* in collisions with other similarly constituted assemblages<sup>6</sup>. In such collisions, energy may be gained or lost. Unless the energy gained exceeds the energy of the bond — as might happen at high temperatures — the atoms of each molecule remain together during and after the encounter. Continuous vibratory recursion is 'the why' of the molecule, *qua* molecule. The fairly complex network of interactions between the four main components of the hydrogen molecule (discussed in exquisite detail by quantum

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5. Vibrational energy is *quantized*. That is, the molecule only absorbs energy of certain specific values.

6. The kinetic energy of the moving gas molecule is proportional to temperature (Kelvin scale).



chemists) that accounts for the minimum in the potential-energy curve for dihydrogen is the main *cause* (in the original Aristotelian sense) of the existence of the dihydrogen molecule. That closed network of relationships is also the basis for the characteristics of collisions between dihydrogen molecules. This collection of relationships is the foundation of whatever efficient causality may be exerted by the moving molecules.

Considered on the basis of the time-scale of human interests, collisions between molecules in a gas at room temperature or above occur rapidly — from our anthropocentric viewpoint, they extend over extremely short periods of time. But electrons within molecules move much more rapidly than relatively ponderous protons do. In fact, it is usually a good approximation<sup>7</sup> to consider that the electrons of a molecule have sufficient time to adjust completely to any motion of atomic nuclei that may occur. On the basis of the time-scale characteristic of *electronic* motions, collisions between molecules are long drawn-out encounters. Since most chemical effects depend on electronic rearrangement, this extension in time of molecular collisions is highly significant for reactivity. The common notion that collisions between molecules are instantaneous should be recognized as an idealization — like a mathematical point with *no* extension — a fiction that is sometimes (but not always) useful. All real interactions, whether they involve molecules or other sorts of entities, are extended in time.

One result of the extension in time of a contact between two particles is that some other significant event may happen *during* the interaction. While the two particles

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7. This is the Born-Oppenheimer approximation.

that are involved in a collision are together, the pair may encounter a third unit. The consequences of the three-particle encounter may well be quite different from the result of any two-particle interaction. The next two sections describe cases in which future events are strongly influenced by persistence of an intermediate aggregate.

### III

The current understanding of the origin of the elements (Cox, 1989) provides a good example of how finite lifetime of a complex species is critical in determining subsequent events. The 'big bang' produced a great deal of hydrogen and helium atoms and relatively minute amounts of  ${}^7\text{Li}$ , a fairly stable (half-life, 53 days) isotope of lithium that has atomic mass of 7. Current understanding is that no atoms heavier than Li were made in the initial processes. Production of the rest of the atoms in the periodic table is generally understood to have required a processing in stars. It now seems quite certain that the initial step in the formation of the heavier elements was production of a beryllium isotope ( ${}^8\text{Be}$ ) that is quite unstable. Like the dihydrogen molecule, the  ${}^8\text{Be}$  nucleus vibrates continually — the relative positions of the eight protons and neutrons that make it up are involved in an elaborate choreography. This fragile nucleus can be produced from the reaction of a proton with  ${}^7\text{Li}$  or, alternatively, by highly energetic collision of two helium nuclei. Once the first stars began burning hydrogen to helium, it became possible to build up enough  ${}^8\text{Be}$  in some stellar interiors that reaction of this fragile nucleus with yet another helium nucleus to yield the stable carbon nucleus,  ${}^{12}\text{C}$ ,

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occurred at a significant rate. Once this bottleneck had been passed, a variety of other transformations came to be possible — production of heavier elements proceeded readily. The complex of factors that accounts for the brief but significant lifetime of  $^8\text{Be}$  (its repeated vibrations about an equilibrium configuration) was critically important for all subsequent events. In the absence of this nucleus,<sup>8</sup> no heavier elements would have been produced.

#### IV

A somewhat less esoteric example of how a short-lived aggregation can control the outcome of a complex process is found in the recent chemical literature. In July, 2000, a news story in a weekly periodical<sup>9</sup> carried the headline "Iridium-catalyzed Process Yields Straight-chain Alkylbenzenes." This report dealt with research (Matsumoto et al, 2000) by a group consisting of scientists from UCLA, Catalytica Inc., and Mitsubishi Corporation, including Roy A. Periana and Henry Taube. For decades, industrial chemists have had effective methods to make branched-chain alkylbenzenes (compounds in which a benzene ring is attached *near the middle* of a hydrocarbon chain). Preparing compounds with a benzene ring *on the end* of a hydrocarbon chain has been much more difficult. Straight-chain products of this hard-to-make type would have specific industrial uses. Devising a practical method to prepare such compounds would

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8. Or another isotope that functioned in a similar way.

9. *Chemical and Engineering News*, July 24, 2000.

be of considerable economic importance. Matsumoto *et al.* invented (or discovered) a catalyst that accomplishes the difficult trick of hooking a benzene ring to the end carbon atom of a hydrocarbon chain. The catalyst works by producing a transient complex that contains two iridium atoms and two benzene rings joined together in a quite specific way. In this intermediate species, each of the two iridium atoms is bound to the side of one benzene ring and, simultaneously, to the flat top of the other benzene ring.

In the reaction mixture in which the catalyst operates, many types of collisions occur. Each of the many kinds of molecules that comprise this reaction mixture collides with all of the other sorts of molecules. For instance, aliphatic (straight-chain) hydrocarbon molecules impact on benzene molecules. But strong bonds hold hydrogen atoms to the six-carbon ring of the benzene molecule. Mere collision with a hydrocarbon molecule will not bring about reaction. However, when a benzene ring is attached to two iridium atoms (as it is in the reaction intermediate produced by this catalyst) rearrangement of the electrons in the molecule weakens some bonds strengthens others. It happens that the reactivity of the hydrogen atoms on the ring is much enhanced. In this situation, reaction with a hydrocarbon molecule that happens to approach from an appropriate direction becomes more probable. The effectiveness of this catalyst — in fostering the reaction of the end carbons of a hydrocarbon chain while not increasing the rate of reaction of the interior carbon atoms — arises from the detailed geometry of the intermediate complex. The peculiar spatial structure of this complex blocks interior carbon atoms of a hydrocarbon chain from approaching the iridium-bound benzene molecules. But end carbons of the hydrocarbon chain are not

prevented from getting to the benzene rings. The reaction does indeed take place by means of a collision of a carbon atom of a hydrocarbon with one of the atoms of a benzene ring, but the specific shape of the intermediate complex selects which minute fraction of the collisions that occur will lead to net chemical change. The vast majority of collisions have no consequences — no chemical reaction occurs. By picking out only those encounters that lead to the more valuable product, and impeding those that, if effective, would have led to the less valuable outcome, this catalyst achieves the result that its designers (or discoverers) desired.

What is the *cause* of the reaction described above? The efficient cause of the production of any particular product molecule is that a specific hydrocarbon molecule happened to collide — with just the right orientation and energy — with a certain benzene ring. The chemical change is indeed brought about by molecular collisions, as the model of causality that we have inherited from the Renaissance requires, but as an explanation this is radically incomplete. The geometric shape of the intermediate complex pre-screens (in a sense) all possible collisions and permits only those that lead to the valuable product. This filtering of events is 'the why' of the process — the reason for the success of the reaction.

That geometric shape is itself the result of the combination of many bonding interactions within the intermediate complex. Each iridium atom is bonded to the edge of one benzene ring by interactions that are similar in many respects to the interactions that hold a dihydrogen molecule together. At the same time, each iridium atom is

attached to the flat top of the other benzene ring — by a bond that is a bit more complicated, but also is similar in some respects to the bonding in dihydrogen. Each of the many chemical bonds in the intermediate complex vibrates, just as the dihydrogen molecule does. The vibrations of these many bonds combine in rather complex patterns — but that does not concern us here. What is important for our purposes is that the effectiveness of the catalyst developed by Matsumoto *et al.* depends on the persistence of one particular intermediate complex, with a specific shape, in the reaction mixture. The particular combination of relationships among the components of this complex that accounts for the stability of this particular intermediate is, in a real sense, the reason (cause in the Aristotelian sense) why the catalyst works as well as it does.

Collisions between hydrocarbon molecules and the intermediate occur with high frequency in the medium in which this reaction occurs. But the vast majority of these encounters are sterile — they do not have consequences. Only a small minority of interactions between molecules have appropriate characteristics (determined by the geometry of the catalyst) to lead to significant results, that is to say, to produce chemical reaction. Many sorts of billiard-ball type collisions occur — but it is the network of inter-relationships among the components of the catalyst that selects which small fraction of these collisions results in chemical reaction. The circumstance that the intermediate benzene-iridium complex vibrates repeatedly around a configuration that is especially reactive is significant for this catalytic reaction, just as the tendency of a dihydrogen molecule to oscillate around its equilibrium position is fundamental to the functioning of H<sub>2</sub> as a molecular unit.

## V

Ilya Prigogine (1999) and his associates in Texas have recently shown that the fact that all interactions are necessarily extended in time presents more than a mere practical problem for the conceptual scheme we have inherited from the era of the scientific revolution. They have shown that when any event (such as an interaction between two particles) extends over a finite time, the result of that interaction cannot, in principle, be predicted deterministically. All predictions of events that follow an interaction that extends in time are *intrinsically* probabilistic. That is, no *real* process follows the deterministic, billiard-ball, efficient causality that the Newtonian synthesis, and current uses of the term cause, assume. Theoretical calculations that generate precise results, based on the use of idealizations such as instantaneous collisions of molecules in a perfect gas, do not provide a reliable basis for investigation of real processes of even moderate complexity. There are sound reasons — theoretical as well as practical — for the conclusion that explanations based only on efficient causality are far from adequate, even for relatively simple problems.

## VI

The systems discussed above all involved collections of *things* (atoms, protons and neutrons, particles in collision). Chemists encounter another sort of coherence — self-organizing collections of *processes*. When chemical systems are far from equilibrium, and involve an autocatalyst (a chemical that increases the rate of its own production) continuous oscillations in chemical concentration are sometimes observed (Ross and

Vlad, 1999). This remarkable result is observed when a process that reduces the concentration of the autocatalyst also occurs in the reaction mixture, and the conditions are such that a complex balance between production and destruction of the autocatalyst is reached. Such systems are called *dissipative structures*.

Chemical reactions that generate oscillations of concentrations can be set up in closed *batch* reactors that do not exchange chemicals or energy with their surroundings, but then the oscillations gradually fade out. In pumped *flow* reactors — open systems that involve continual addition of and removal of material<sup>10</sup> — oscillations can persist indefinitely. Pumped systems often have two *non-equilibrium steady states*. One of these steady states (let's call it blue) has a high autocatalyst concentration: it occurs if pumping is slow. At high rates of pumping, a different steady state (call it red) with a low autocatalyst concentration exists. At intermediate pump-rates, both of these non-equilibrium steady states can become *unstable*, and oscillations may occur. Oscillation involves repeated shifts from something close to the red state to a condition similar to the blue state, and then the reverse transition.

As long as conditions remain favorable, concentrations of all the chemical components of chemical dissipative structure continually rise and fall — tracing out the same<sup>11</sup> set of states in each oscillation. Within limits, such systems may be remarkably

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10. Similar results can be achieved by irradiation by light.

11. In systems that demonstrate *chemical chaos*, the oscillations do not follow a single closed set of states (a limit cycle) but rather they remain on a 'strange



resilient, oscillations continuing with only minor change under considerable variation of conditions. This inherent flexibility allows the reaction system to maintain its integrity while interacting with the rest of the world. In this respect, the oscillation of the pumped system is similar to vibration of the dihydrogen molecule, the basis for that molecule's integrity in collisions. So long as the constraints mentioned above continue to be met, the dissipative structure continues to exist, and that structure, as an integral unit, may serve as a center of agency. Interactions<sup>12</sup> of the system with the rest of the world are quite different in the presence of the dissipative structure than they would be in the absence of that self-organized coherence. In this sense, the closure of a network of relationships that gives rise to a dissipative structure (Earley, 2000) is the 'unit-determining' feature required to secure 'unithood', in D. M. Armstrong's (1997) terminology.

The mathematical scheme used to model the simplest chemical oscillation in a pumped system is the same as the model generally used to understand the generation of

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attractor' — they follow a sequence of states that repeats approximately, but not exactly.

12. The effects of the structure as whole are the resultant of the effects of the components, but the concentrations of the components that exist at any instant are the effects of the *closure* of the limit cycle. This is a definite example of a kind of 'downward causation,' — an influence on the components arising from the thing those components constitute.

calcium oscillations in biological cells. (Goldbetter, 1996) These oscillations are known to function in the control of complex biological organs, such as the human brain (Putney, Jr., 1998). Remarkably, it is the frequency, not the amplitude of the calcium oscillations that is decoded as the controlling signal (DeKonnick and Schulman, 1998). The signal is generated by the unit-determining *closure* of the regulatory network that defines a kind of dissipative structure composed of processes in the brain. The information that is transmitted results from subtle alteration in the parameters that control that oscillation. There seems to be no way to deal with effects of this sort using efficient causality alone. The restriction of causality to efficient factors (and the concomitant de-emphasis of structural features) is highly problematic in dealing with the closures of relationships that account for dissipative structures. As Juarrero points out, difficulties of this sort are of central significance in questions of philosophy of mind and of human action, but their outline seems clear even in the simpler chemical cases discussed in this paper.

## VII

Situations where *closure* of a network of processes has important effects occur in many fields. In systems involving electrons and atomic nuclei, there are stringent conditions on the *closure* of sets of relationships. Once that closure is attained, a system maintains its coherence indefinitely, and can function as a unit in yet higher-level coherences. The postulate of de Broglie, central to the development of quantum mechanics, is strikingly similar in some respects to the positions being advocated here. Networks of interaction

also abound in biochemistry, molecular biology, organismic biology, and ecology — as well as in economics and the areas studied by the social sciences. In favorable cases, systems in all these areas display 'unit making' closure of relationships quite similar to those displayed by dissipative structures.

Elsewhere (Earley, 1998), I have applied the concepts outlined here to some major problems of philosophy; the same approach can also be applied to the kind of paradoxical questions that many philosophers of science enjoy discussing. David Lewis (1993) considered two instances of 'the problem of the many' that were raised by Peter Unger (1980). One is the question of the identity of a cloud in the summer sky — from a distance, each cloud seems to be a unit, but on closer examination it is found to be merely an ill defined heap of small water droplets. The point of view adopted here calls attention to the set of rising and falling air currents that defines each isolated cumulus cloud. It is the (unit-determining) *closure* of such cycles (convection cells) that gives the cloud the limited identity it has. Unger's second question deals with Tibbles, a shedding cat (on a mat, of course). Is there just one cat or are there 1001 cats, each differing from the others by one or more cat-hairs? The present viewpoint holds that Tibbles, like other living organisms, is defined by closure of a large number of internal networks of biochemical interactions (metabolism, respiration, etc.). Each of these closures is more complicated than the simple dissipative structures we have been discussing, but shares 'unit-determining' features with them. There is just one complete set of such closures, not 1001.

What needs to be added to our current understanding of causation? All of the examples given above involve efficient causation, but this alone is radically insufficient to *explain* the phenomena — to lead to an understanding of the *reasons* behind the events. Efficient causality, alone does not illuminate 'the why' of the topic under investigation. In each of the three cases discussed, relationships between components are critical — but it is the peculiar *closure* of these sets of relationships that defines the coherence. Closure of set of relationships is itself a higher-level relationship — what used to be called a *form*. The notion of *formal cause*, was extruded from philosophy at the Renaissance. Scientists, and technologists, unblushing opportunists as they are, have continued to use notions similar to formal cause, under the designation *structure*. This way of thinking tends to favor the opinion that structure results from efficient causes. The examples given above show that the reverse is often the case. Often, the structure (formal cause) of a situation determines which small fraction of many possibly efficient factors are actually effective.

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