Essays in the Philosophy of Chemistry

Edited by ERIC SCERRI AND GRANT FISHER

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Introduction

ERIC SCERRI AND GRANT FISHER

The chapter by Joseph E. Earley Sr. (chap. 10) can only be described as a tour de force in every sense of the term. Earley's writing, perhaps more than that of any other currently active author, displays a complete mastery of both the philosophical and the chemical literature. Nothing that could be said briefly here would do justice to his essay, which ranges across a diverse set of topics including the nature of substance, properties and relations, bundles, molecular properties, onticity, wholes and parts and much more.

CHAPTER 10

How Properties Hold Together in Substances

JOSEPH E. EARLEY, SR.

1 *What Has Chemistry to Do with Philosophy?*

A main aim of chemical research is to understand how the characteristic properties of specific chemical substances relate to the *composition* and to the *structure* of those materials. Such investigations assume a broad consensus regarding basic aspects of chemistry. Philosophers generally regard widespread agreement on basic principles as a remote goal, not something already achieved. They do not agree on how properties stay together in ordinary objects. Some follow John Locke [1632–1704] and maintain that properties of entities *inhere in substrates*. The item that this approach considers to underlie characteristics is often called "a bare particular" (Sider 2006). However, others reject this understanding and hold that substances are *bundles of properties*—an approach advocated by David Hume [1711–1776]. Some supporters of Hume's theory hold that entities are collections of "tropes" (property-instances) held together in a "compresence relationship" (Simons 1994). Recently several authors have pointed out the importance of "structures" for the coherence of substances, but serious questions have been raised about those proposals. Philosophers generally use a time-independent (synchronic) approach and do not consider how chemists understand properties of chemical substances and of dynamic networks of chemical reactions.

This chapter aims to clarify how current chemical understanding relates to aspects of contemporary philosophy. The first section introduces philosophical debates, the second considers properties of chemical systems, the third part deals with theories of wholes and parts, the fourth segment argues that *closure* grounds properties of coherences, the fifth section introduces *structural realism* (SR), the sixth part considers contextual emergence and concludes that *dynamic structures of processes* may qualify as *determinants* ("causes") of specific outcomes, and the final section suggests that ordinary items are based on *closure of relationships* among constituents *additionally determined* by selection for integration into more-extensive coherences.

1.1 Substances

Ruth Garrett Millikan discussed the concept of *substance* in philosophy:

> Substances . . . are whatever one can learn from given only one or a few encounters, various skills or information that will apply to other encounters. . . . Further, this possibility must be grounded in some kind of natural necessity. . . . The function of a substance concept is to make possible this sort of learning and use of knowledge for a specific substance.
>
> (MILLIKAN 2000, 33)

Substances necessarily persist through time and thus are distinguished from events. Chemists, however, define chemical substances as materials of constant composition and definite properties—and also consider all systems to be composed of smaller items. They hold that macroscopic samples are made up of molecules and that molecules have atomic nuclei and electrons as components. All of these bits are in incessant motion, and in continual interaction with other items. The long-term stability of composite chemical entities implies that internal motions are *somehow constrained* so that the composites retain integrity over time and through interaction. Paul Weiss described this situation in terms of the philosophers' concept of substance:

> Each actuality is a substance. It maintains a hold on whatever it contains, produces, and intrudes upon. It persists and it acts. It has an irreducible, independent core, and receives determinations from insistent, intrusive forces. . . . If an actuality were not a substance, its parts would not belong to it, and it would disperse itself in the very act of making its presence evident. The very items which it dominates, it would not control; nor would it continue to be despite an involvement in change and motion. It would be inert and solely in itself, or it would be a mere event. In either case, it would not be a source of action.
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> (WEISS 1959, 109)

The well-established dynamic aspect of nature requires attention to how properties of chemical entities are maintained through time, and how they maintain integrity during interaction. Failure to consider factors involving time (use of *synchronic* rather than *diachronic* approaches) is not acceptable (Humphrys 2008, 1997; Earley 2012b).

1.2 Properties and Relations

Natural human languages function *as if* all items fall into one or the other of two great classes: *subjects* (substances, particulars, or individuals) and *predicates* (attributes or universals—including properties and relations). Aristotle's early definition: "A substance . . . is that which is neither said of a subject nor [is] in a subject" (*Categories* 5 (2^b, 13–14), Barnes 1984, 4) is similar to Bertrand Russell's characterization: "An 'individual' is anything that can be the subject of an atomic proposition" (Russell's "Introduction" in Whitehead and Russell 1970, xix).

Russell considered that whatever can be truly asserted concerning an individual (any predicate whatsoever) is a property (attribute) of that particular. Hilary Putnam (1969) pointed out that philosophers who use such broad understandings often run into difficulties that use of narrower property-concepts would avoid. D. H. Mellor (2006) conceded real existence only to those properties and relations that science discovers to be involved in causal laws and argued that many generally-accepted properties (including redness) *do not exist*—because any causal regularity can be dealt with without recognizing them.

Chemists generally use a restricted notion of property which was described by American chemist and philosopher Charles S. Peirce [1839–1914]—that is, a property is *how a thing behaves, or would behave, in a specified operation* (CP 8.208).[1] This usage exemplifies Peirce's Pragmatic Maxim: "Consider what effects, that might conceivably have practical bearings, we conceive the object of our conception to have. Then our conception of these effects is the whole of our conception of the object" (CP 5.402). We follow the usual practice of chemists and use Peirce's concept of property.

Properties filling either Mellor's or Peirce's property-concepts (including powers, capacities, vulnerabilities, and affordances) are classed as dispositional properties. Non-dispositional properties are designated as categorial or substantive properties. *Intrinsic* properties are distinguished from *structural* properties—features of entities that depend on relationship(s). *Relations* involve two or more individuals as *relata*. Some claim that many-place (polyadic) relations can be *reduced to* single-place (monadic) properties. But Russell argued that *unsymmetrical* relations such as *greater than* cannot be reduced to monadic properties.

In the mid twentieth century some held that all problems could be understood in terms of non-composite entities (elementary particles) with intrinsic properties. An alternative view is that every apparently-intrinsic property derives from *interaction* of less extensive components—as the mass of the proton mainly arises from *the combination* of its three component quarks, not from their intrinsic masses (Dürr, Fodor, Frison,Hoelbling, Hoffmann, Katz, et al. 2008). On the former view, intrinsic properties are primary and structural (relational) properties secondary: on the alternative basis structural properties are fundamental.

1.3 Alternatives to the Substance-Attribute Approach

Alfred North Whitehead held that: "All modern philosophy hinges round the difficulty of describing the world in terms of subject and predicate, substance and quality, particular and universal" (Whitehead 1978, 49). Whitehead *rejected* Locke's category of substance and asserted: "'Actual entities'—also termed 'actual occasions'—are the final real things of which the world is made up" (18). *Process* for Whitehead is all of a single sort—self-creation of actual occasions.

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[1] Paragraph 208 of volume 8 of the electronic version of *The Collected Papers of Charles Sanders Pierce*. Further citations to this work will follow this style.

"Actual entities perish, but do not change; they are what they are" (35). Actual occasions are not substances—they come to be and, in so doing, perish.

Donald W. Mertz (1996, 2003) avoids the substance-property distinction in a different way. Mertz's "Instance Ontology" operates with a single ontological category—called property instance, state of affairs, or fact of relationship. By recognition of intension-types (universals), Mertz's approach qualifies as realism. Each state of affairs corresponds to *unification* of its relata. Gilbert Simondon recommended that we should "seek to know the individual through individuation rather than individuation through the individual" (Simondon 1964, 22). Whitehead made the *achievement* of individuality by each actual occasion a focus of his system. Mertz does not deal with the *process* of individuation.

1.4 Substrate-Bundle Debates

Locke admitted that the concept of substratum was "only a supposition of he knows not what support" of properties (1690, chapter XXIII, section 2): in an Appendix to his *Treatise*, Hume (1739) reported: "I am sensible, that my account is very defective." In the end, Hume was as dissatisfied with his bundle approach as Locke had been with his substratum theory: Present-day advocates of either approach rarely express similar reservations.

Jiri Benovsky (2008) examined several versions of both substrate and bundle theories—some involving tropes and others recognizing universals, some with a single identical unification-relation for all objects, others with variable numbers of relata (*polyadicity*), and still others with distinct unification-relations for each object. Benovsky considered how proponents of each of these versions defended against objections and concluded that both substratum and bundle theories *share a common central postulate*—the concept that each object has a unifying feature. (This is the substrate/bare particular or the compresence relationship.) He identifies these as *theoretical entities* (items "individuated by their theoretical role") and points out that all "play the same role in the same way" in all their applications—therefore they are "identical (*metaphysically equivalent*)" (183). He concludes that substratum and bundle theories are twin brothers not enemies—and that both are seriously deficient, since neither has clarified the unification that they both require. That unification remains a "something, he knows not what" as it was for Locke: both substrate and bundle approaches are still "very defective" as Hume found his own theory to be.

1.5 A Proposed Principle of Unity for Bundles

David Robb (2005, 467) described an explicit search for a *principle of unity* for properties. A certain tennis-ball (called Alpha) figures in these discussions. Robb begins:

> It's hard to deny that there are *natures* or *ways of being*.... How could there be being without a way of being? To be is to be some way or other. I'll call these ways *properties*.... Ordinary objects (chairs, trees, human beings, electrons, stars)...are merely bundles of properties. Not only must a being be some way or other, it is *exhausted* by ways of being.

Robb holds that an object (such as Alpha) "is a unified, persisting, independent being" (468) but does not examine the basis of such unity, persistence, and independence. Although he considers that objects necessarily persist, Robb specifically states "I will not address diachronic unity here" (476). His treatment is synchronic. Robb states: "Whether something counts as an object may for the purposes of this paper be taken as a primitive fact about it" (468). Elsewhere (Robb 2009) he expands on various aspects of notions of substantiality—but does not propose a criterion of what unifies an object. He holds that parts of objects that are themselves objects are substantial parts: parts that are properties (rather than objects) are qualitative parts. Each object has both substantial and qualitative unity—these are distinct, but "we should expect there to be some systematic relations between them such that our choice of one constrains our choice of the other" (474).

Robb declines to express an opinion as to what the principle of unity of substantial parts might be since: "My concern here in defending the bundle theory is only with the principle of qualitative unity" (474). He uses David Armstrong's concept of a *structural* property: "a kind of complex property, one composed of the properties of and, in most cases, relations among [an] object's parts" (476). Adding: "to say that certain substantial parts are *exhaustive* at a particular mereological[2] level means that those parts are *all* of an object's parts at that mereological level" (477), he proposes a *qualitative principle of unity:*

> (CU) For any substantially complex object **O** and properties F and G, F and G are qualitative parts of **O** iff F and G are both structured on the (exhaustive) substantial parts of **O** at some mereological level.

That is to say, if an object has parts that are themselves objects, then the properties of the composite object are some combination of the properties of the parts—providing that all the parts identified at a particular mereological level are taken into account. Those resultant object-properties may be regarded as parts of the object, but they are parts in a qualitative sense that is different from the usual (substantial) sense of parthood. Robb assumes that the properties of ordinary objects derive directly and exclusively from the properties of their components.

The principle of unity (CU) does not apply to simples—objects that have no substantial parts. Robb presumes that simples exist and invokes the principle that "if no objects exist in their own rights then no objects exist at all" (485). Robb proposes: "A simple object...just *is* a single, simple property" (486) and formalizes that assertion as:

> (SU) For any substantially simple object ***O*** and properties F and G: F and G are *qualitative parts* of ***O*** iff F and G are each identical with ***O***.

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[2] Mereology is defined as "the abstract study of the relations between parts and wholes" [*Shorter Oxford English Dictionary, Volume I.* (1993). Oxford: Clarendon Press, 1747]. See section 3.1 of this chapter.

Robb argues vigorously that SU does not involve the category-mistake of confounding (adverbial) ways of being with (substantive) entities, but observes that if SU does involve a category-mistake then "it's one that bundle theorists have been making all along" (486).

2 *Properties of Chemical Systems*

Some characteristics of chemical systems (called *molecular* properties) depend mainly on the characteristics of components of those systems together with how those constituents are connected. In contrast *spectroscopic properties* involve *transition* between energy states of entities—with concomitant emission or absorbtion of energy. *Chemical properties* involve interaction of substances with like or different others to bring about transition to alternative compositions—thereby producing new *connectivities* (three-dimensional arrangements) of elemental centers ("atoms"; Bader and Matta 2013).

2.1 Molecular Properties

In chemical entities, attractive forces (such as between unlike electrical charges) pull components together; repulsive interactions (as between like charges) drive constituents apart. As parts separate, attractive forces draw fragments together. Distances between components change continuously, but remain within limits—due to *balance* of attractive and repulsive interactions. *Closure* of relationships enables each chemical entity to retain self-identity through interactions.

Molecules adopt the spatial configuration with lowest potential energy that is consistent with constraints which obtain. For dihydrogen, a minimum of potential energy occurs at *a single* internuclear distance (the H–H bond-length). More-complex chemical entities are described in multidimensional configuration space. Potential-energy minima in configuration space correspond to more or less stable molecular structures: the minimum of lowest energy is the equilibrium structure (Earley 2012b). Vibrations around such structures occur, and are more vigorous at higher temperature. Stability corresponds to *closure of relationships among components* which leads to *a minimum of potential energy* for a specific connectivity of elemental centers. The details of each such "potential-well" determine how each system interacts, and specifies many properties of the coherence. Closure of relationships of components is what accounts for the coherence of diverse properties for each molecular substance. Such closure allows each molecule *to make a characteristic difference* and so have ontological significance (Earley 2008a, Ney 2009).

The factors that determine the variation of potential-energy with internuclear distance for the dihydrogen molecule are well understood. Electrostatic attraction between negatively-charged electrons and positively charged protons, mutual repulsion of like-charged electrons (and protons), the fact that the internal energy of atoms and molecules is restricted to certain specific values (quantized), and the Pauli Exclusion Principle (which limits occupany of each molecular energy-level to two electrons) are all major factors. For the dihydrogen molecule, theory-based (a priori) calculations of molecular properites—dissociation energy, equilibrium internuclear distance, rotational moment of inertia—agree well with experimentally-determined values. Approximate calculations for more-complex molecules—usually involving parameters estimated from experiments—yield approximate predictions of characteristics of chemical molecules, even for some quite complicated ones.

Properties that depend only on the mass and/or volume of molecules derive directly from phenomena that potential-energy–versus–internuclear-distance curves describe. Certain (colligative) properties of solutions depend on the *number* of solute units (molecules or ions) dissolved in a given volume of solvent, rather than on the properties of the individual molecules. Properties such as the melting temperature of a solid, the boiling temperature of a liquid, the critical temperature of a substance all depend on mutual interaction of molecules of a single type. Both colligative and phase-change properties might well be grouped with molecular properties.

2.2 Spectroscopic Properties

Like electronic energies, vibrational and rotational energies are *quantized*. Possible energy-levels are separated more widely for electronic states, less widely for vibrational states, and quite narrowly for rotational states. Transition from one energy level to another involves absorption or emission of energy. If a dihydrogen molecule (H_2) absorbs a photon of appropriate energy, a transition from a lower-energy electronic level to a higher-energy electronic level would occur. Once the system was in the upper level (with a longer equilibrium-distance) vibrations and rotation could occur but sooner or later either a photon would be emitted and the molecule would relax to the lower level, or the molecule would split to produce energetically-excited hydrogen atoms. Transitions between energy levels provide a way by which molecules interact with the rest of the world while retaining integrity (for dihydrogen, by maintaining the H-H bond). Under usual conditions, some chemical coherences persist indefinitely, others have short lifetimes, and many are evanescent. Arguably, persisting long enough to undergo rotation is the lower-limit of molecular existence (Earley 1992).

The geometric structures of molecules and crystals partially determine their spectra. Details of structure can often be inferred from spectral measurements. *Spectroscopy*—study of the energy absorbed or released when chemical systems change from one energy level to another—accounts for much of the effectiveness of modern chemical science.

2.3 Chemical Properties

Chemistry turns less-valuable materials into more-valuable items. When materials are mixed, new substances appear and old ones vanish as component elementary centers rearrange. Every reaction involves a *decrease* in free energy—a lowering of potential for chemical reaction. Reaction continues, however slowly, until a minimum of free energy is reached—at a condition of chemical equilibrium—and no further net change occurs although forward and reverse reactions continue at equal rates.

Any given starting mixture conceivably could produce a variety of final products. Principles governing alternative changes are easy to state: Applying them requires experience and skill. The two main considerations are *thermodynamic stability* and *kinetics* (speed). If all reactions occur rapidly, the final state will be the condition that has the lowest free energy—total energy decrease due to chemical bonding adjusted to take account of the complexity of the structures involved (less-complicated structures have an advantage over more-complex ones). Every chemical change involves decrease in thermodynamic reaction-capacity of the system—reduction of free energy or chemical potential. Chemical reaction corresponds to transition between stable states—movement of a system from one potential-well to another. Chemical reactions correspond to production of new closures—every chemical process is a becoming (Earley 1998).

Transition from reactant to product potential-wells necessarily involves passage through higher-energy arrangements of components which are *intermediate* between the configurations of the starting materials and products. *Slower* rates of chemical reaction involve traversing patterns corresponding to higher potential-energy barriers between reactant and product potential-wells: faster reactions involve lower barriers. For instance, change from the stable *cis*-conformation of 1,2-dichloroethane ($C_2H_6Cl_2$) to the equally-stable *trans*-configuration of the same molecule occurs rapidly. The corresponding reaction of 1,2-dichloroethylene ($C_2H_4Cl_2$) is slower because the stronger double bond between carbon centers resists twisting.

It is a serious error to focus only on *thermodynamic* factors and to ignore *kinetic* (reaction-rate) considerations. Most chemically interesting reactions are *controlled* by kinetic influences, so that history must be taken into account. Quite usually, the product that results from a chemical change is not the thermodynamically most stable product but some higher-free-energy form(s) (Earley 2012b).

Rates of chemical reactions are usually discussed *as if* intermediate "transition" states had real existence. This approach forms the basis of a myriad of chemical explanations of widely varying sophistication. Eugene Wigner suggested that reaction-rate parameters should be computed directly from molecular dynamics, as a preferable alternative to the thermodynamics-related transition-state approach to understanding reaction rates (Jaffé, Kawai, Palacián, Yanguas, and Uzer 2005). Molecular-dynamics calculations can now compute the motions of some tens of individual atoms during reaction. For instance, modeling of the isomerization of HCN to produce HNC (Ezra 2009) shows that quasi-periodic trajectories and multidimensional chaos exert significant influences on chemical reactivity. The transition-state approach does not take account of such effects: To the extent that they are important that approach may lead to wrong conclusions.

Typically, chemical reactions happen through several rather distinct subprocesses, which often involve intermediates of significant stability. Such a series of steps is called a *reaction mechanism*. The reaction rate for each such mechanistic step is subject to many influences, generally different for each step. Sometimes, one step will be so much slower than the others that it will *mainly determine* the overall reaction rate but usually several reaction steps will be significant for determining the overall rate of reaction.

It sometimes happens that reaction-rates for a series of related reactions follow the trend in thermodynamic driving-force (free energy) for the same series—but *there is no necessity* for this to be the case. Reactions with highly favorable free-energy changes may well be slow; reactions with low thermodynamic driving-force might be rapid. *Which product* (of the myriad possible in a particular case) results from a mixture of reactants is usually determined by the relative rates of *many competing reactions*. Rarely does a collection of starting materials generate a single product: usually several products occur in proportions which depend sensitively on environmental conditions. Large networks of reactions (such as occur in biochemistry, astrochemistry, or geochemistry) are governed by the relatively-simple principles just summarized but each type of reaction-network has additional special features.

2.4 Relative Onticity

Early in the twentieth century, a disagreement between physicists attracted attention (Atmanspacher and Primas 2003, 301). Albert Einstein held: "Physics is an attempt conceptually to grasp reality as it is thought independently of its being observed." In contrast, Niels Bohr warned: "It is wrong to think that the task of physics is to find out how nature is. Physics concerns what we can say about nature." It became customary to distinguish scientific statements as either *ontological* or *epistemological*. The former deal with how things *really are*: the latter concern how things *appear to be*. Eventually most scientists came to assume that only the a priori calculations of quantum physics merited the ontological designation. Admixture of a posteriori considerations was considered to relegate a statement to mere epistemological status. The opinion that chemical propositions *could not attain* to ontological status became widespread: this view still has adherents (e.g., McIntyre 2007). But this clear position is subject to Putnam's objection:

> Once we assume that there is, somehow fixed in advance, a single 'real,' a single 'literal' sense of 'exist'—and, by the way, a single 'literal' sense of identity—one which is cast in marble and cannot be either contracted or expanded without defiling the statue of the god, we are already wandering in Cloud Cuckoo Land.
>
> (PUTNAM 2004, 84)

Chemists believe that they clarify the *real order of things* when they provide detailed accounts of the diverse chemical species with which they deal. But they employ a multi-level system of entities (Earley 2003b)—they use a *relative* *onticity*. Which levels of entities are to be employed in a discourse is decided *during* the formulation of the discourse—not in advance, as many logical systems assume.[3]

> The distinction of epistemic and ontic descriptions can be applied to the entire hierarchy of (perhaps partially overlapping) domains leading from fundamental particles in basic physics to chemistry and even to living system in biology and psychology. Ontic and epistemic descriptions are then considered as relative to two (successive) domains in the hierarchy.... While atoms and molecules are epistemically described within the domains of basic physics they acquire ontic significance within the domain of chemistry... the central point of the concept of relative onticity is that states and properties of a system which belong to an epistemic description in a particular domain can be considered as belonging to an ontologic description from the perspective of another domain.
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> (ATMANSPACHER AND PRIMAS 2003, 311)

3 *Coherence*

3.1 Wholes and Parts

According to the dictionary definition given in note 2 any theory of wholes and parts is "a mereology." However, the specific part-whole logical system that Peter Simons (1987, 1) calls Classical Extensional Mereology (CEM) has influenced English-speaking philosophers so deeply that that 'mereology' often refers exclusively to CEM. Three basic axioms of CEM (Lewis 1991, 74) are

Transitivity: If x is part of some part of y, then x is part of y.

Unrestricted Composition: Whenever there are some things, there exists a fusion of those things.

Uniqueness of Composition: It never happens that the same things have two different fusions.

The first axiom is relatively non-controversial: The knob of a door in a house is a part of the house. The second axiom seems troublesome, since it gives rise to statements such as that of Willard V. Quine: "There is a physical object part of which is a silver dollar now in my pocket and the rest of which is a temporal segment of the Eiffel Tower through its third decade" (Quine 1976, 859). However Quine also states:

> Identification of an object from moment to moment is indeed on a par with identifying an object from world to [possible] world: both identifications are vacuous, pending further directives.... The notion of knowing who someone is, or what something is, makes sense only in the light of the situation. It all depends on what more specific question one may have had in mind.
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> (QUINE 1976, 863)

One can understand this as giving the axiom of unrestricted composition a *pragmatic* interpretation: what sorts of items should be in a universe of discourse depends on the *purpose* of the discussion—if it should be useful in some particular inquiry, any grouping of items might properly be taken to comprise a single unit. On that interpretation, the principle of unrestricted composition would be acceptable, but with an odd notion of existence.

The third axiom of CEM (uniqueness of composition) clearly is incompatible with chemical understanding. *Normal butane*, $CH_3CH_2CH_2CH_3$, and *isobutane* $(CH_3)_3CH$, have quite distinct properties but identical atomic-level constituents (C_4H_{10}). This is precisely what the third principle of CEM asserts *does not occur*. CEM is clearly *not appropriate* for *chemical* wholes and parts.

William Wimsatt identified "four conditions [that] seem separately necessary and jointly sufficient for *aggregativity* or non-emergence"—the situation in which the axioms of CEM might apply. One is *absence* of cooperative or anti-cooperative interactions: any such nonlinearity would make CEM inapplicable. The other three conditions require *invariance of all system-properties* under certain operations: (1) rearranging the system parts, (2) decomposing the system into its parts and then recombining the parts to reconstitute the system, and (3) subtracting parts of the system or adding more similar parts. If operations (1) or (2) result in any change—or there is a *qualitative* change under operation (3)—then the system is not a mere aggregation and CEM *cannot* apply. Wimsatt concludes: "*It is rare indeed that all of these conditions are met*" (Wimsatt 2006, 675, emphasis in original).

Wimsatt developed a trichotomy in which *aggregates* (to which CEM may apply) are clearly distinguished from *composed systems*, in which details of connectivity (in what ways components relate to each other) strongly influence the characteristics of the system, and a third class is *evolved systems*—those that have developed through historical selection processes so that no way of identifying component parts has priority. In such systems, there is no unambiguous way to determine what the *parts* of the composite system are: investigations carried out for diverse purposes will identify different items as parts of the system. Investigators who prefer to deal with decomposable coherences avoid such systems—but that does not show that they are either unimportant or uninteresting. Chemical systems are composed systems rather than aggregates: Biological and ecological systems generally fall in the evolved-systems category. Since atoms of most chemical elements were generated by contingent processes in exploding stars, chemical entities might also be properly regarded (for some purposes) as evolved systems.

Philosophical discussions generally assume (e.g., Robb 2005, Vander Laan 2010), often implicitly (Armstrong 2010), that items do not change when they become parts of wholes—so that there is no ambiguity in identifying which individuals are the parts of a composite whole. Chemical and biological experience clearly indicates that entities included as parts of compound individuals

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[3] Ruth Barcan Marcus (1963) proposed a *substitutional* interpretation of first-order logic: This interpretation does not require specification of a universe of discourse in advance but rather admits all *entities that figure in true statements*. Her interpretation (also called "truth-value logic") should be more appropriate for chemical inquiry than is the standard ("objectual") logical approach.

are greatly changed by their inclusion in such wholes. Items included in coherences often (but not always) retain their individuality—but their properties in the whole are generally not the same as the characteristics of similar items outside such coherences.

Simons (1987) pointed out that the Polish logicians from whose work CEM derives had strong prior commitments to nominalism—the doctrine that *only individuals* actually exist—and that therefore they eschewed recognition of universals (properties and relations). Contemporary nominalists (e.g., Lewis 1991) also regard universals as no more than linguistic conveniences. For them, only particulars *really* exist. In contrast, *ante rem* (or Platonic) realists—perhaps including David Armstrong (2010)—hold that properties and relations, although they are not located in space or time, *really exist* independently of (and in some sense prior to) the individuals that constitute instances of those universals. Several positions (jointly designated moderate or *in rem* realism) are intermediate between nominalism and *ante rem* realism: they typically hold that properties and relations are important—but they only exist as *features of individuals*. Kit Fine (2006) and Kathrin Koslicki (2008) endorse the notion that arrangements of components—structures—are essential to the coherence of objects, and therefore structures should be considered *proper parts* of objects. There is an urgent need for formal development of alternative mereological systems[4] that will have wider applicability than CEM does (Llored 2010, Harré and Llored 2011).

David Vander Laan (2010, 135) reports that the question "'Under what conditions do some objects compose another?' has increasingly been recognized as a central question for the ontology of material objects." This query (known as "the composition question") consists of two sub-questions:

1. How can several items *function as a single unit* in causal interactions?
2. What characteristics must individuals have in order to constitute such a causally-effective unit?

The first is the external (or *epistemological*) sub-question: the second, the *ontological* sub-question.

3.2 Symmetries and Groups

Three of Wimsatt's four conditions for aggregativity involve *invariance of system properties under a specified operation*. This characteristic of a system is called

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[4] A. N. Whitehead sketched out an alternative mereology even before CEM was developed (Simons 1987, 81–86). Whitehead based his system on an insight that he later summarized as: "However we fix a determinate entity, there is always a narrower determination of something which is presupposed in our first choice, also there is always a wider determination into which our first choice fades by transition beyond itself" (Whitehead 1967, 93). This can be stated more formally as: *for every particular x there exists an entity y that extends over x, and there also exists an individual z that x extends over.* Whitehead did not complete development of his mereological system, but his basic approach seems more consistent with chemical practice and its results than is CEM. Both Whitehead's multi-level mereology and Ruth Barcan Marcus' substitutional logic can accommodate the importance of *purposes* in scientific representation.

symmetry. Wimsatt's conclusion can be rephrased as: CEM applies if the system of interest involves *neither* cooperative or inhibitory interactions, and *also* is *symmetric* with respect to *all three* of the operations, (1) rearranging constituent parts, (2) disassembling and reassembling those fragments, and (3) adding components similar to those already present, or subtracting some of the original parts. Systems to which *all four* of these conditions apply are *extremely rare*.

Symmetry conditions such as Wimsatt invokes are at the center of currently-used tests for the identity of entities. Galileo Galilei's seventeenth-century research led to general and explicit acceptance of the uniformitarian doctrines that physical laws are the same in all parts of the universe, that all times are equivalent, and that no spatial direction is preferred. On this basis, physical objects can properly be described at any specific time (past, present, or future) and using any convenient coordinate system (oriented in any direction). Since Galileo also established that acceleration (rather than velocity) is what is important, objects can be represented as moving with respect to an external reference point at any constant velocity. (This is the Galilean principle of relativity.) On this basis, the validity of a description would not change on alteration of the single time specification, the three spatial coordinates, the three orientation angles, or the three velocity components (boosts). Any entity that is not changed by any of these ten transformations (alone or in combination) is considered to be a Galilean particle (Castellani 1998)—that is, such a coherence is properly regarded as a *single individual existent*.

Each of the entities considered in current particle-physics displays *symmetries* (invariance under appropriate operations) that correspond to (represent) one or another of certain mathematical objects called *groups*. A group is a special kind of set (a collection of elements) for which applying a stated procedure (the group operation) to any two members of the group generates a *member of the group*—and not something else. This closure requirement is a severe one: Groups are rare among sets (Joseph E. Earley 2013).

The ten operations under which Galilean particles are symmetric (single time-specification, three spatial coordinates, three orientation angles, and three velocity components) constitute the defining operations of the Galilei Group, designated G. Each of the many types of Galilean particles corresponds to a representation of G. Since all the component operations of G can be carried out to greater or lesser degrees without restriction (like the rotations of a circle about its center), G is a continuous group rather than a discontinuous or discrete group. (Rotation of a regular polygon around its center corresponds to a discrete group.)

3.3 Extensions of the Symmetry Concept

In 1929 Hermann Weyl revived a proposal he had made in 1918 that descriptions of electromagnetic systems would be unchanged by a gauge transformation—an operation by which λ, the phase[5] of the wave function ψ, was changed

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[5] The fraction (say, 45°) of the complete (360°) oscillation completed at a given instant.

by an amount that differed in various locations ($\lambda = \lambda(x)$)—and a corresponding term was added to the electromagnetic potential f_p.[6] With respect to this transformation, Cao observed:

> In this way the apparent 'arbitrariness' formerly ascribed to the potential is now understood as freedom to choose any value for the phase of a wave function without affecting the equation. This is exactly what gauge invariance means.
> (CAO 1988, 120)

By 1927 Wolfgang Pauli had rationalized Pieter Zeeman's 1896 discovery that magnetic fields *split* spectral lines, on the basis of the proposal that electrons possessed intrinsic angular momentum (spin): he also explained the 1922 demonstration by Otto Stern and Walther Gerlach that magnetic fields split beams of silver atoms, by postulating that silver ions also had spin. In 1928 Paul Dirac rationalized the spins of the electron and of the silver ion by combining gauge transformations with Einstein's Special Theory of Relativity. The Poincaré Group—the product of the ten operations that define the Galilei group G and the four Lorentz transformations[7]—defined each particle, as the Galilei group had done in ordinary mechanics.

After the neutron (discovered in 1932) turned out to be nearly identical to the proton (except for electrical charge), Eugene Wigner (1937) proposed that the proton and neutron should be regarded as *alternative energy states* of a single particle-type—resembling the two (+½ and –½) spin-states of the electron. He suggested the name isospin for whatever characteristic of these entities might be analogous to electron spin. Isospin, so conceived, does not have units of angular momentum as electron spin does—the name is *clearly metaphorical*. In 1954, after the detection of other subatomic particles, Chen Yang and Robert Mills proposed that the proton, the neutron, and other hadrons should be considered to be interrelated by gauge symmetries involving isotopic spin (also called isospin or, preferably, isobaric spin) which could assume values including ½, 1, and 3/2. This approach predicted the existence of a number of previously-unknown particles that subsequently were experimentally observed.

It turns out that the symmetries corresponding to the electronic spin and isobaric spin are *not* continuous, as are direct coordinate transformations. For instance, there are *only two* values of electronic spin (+½ and –½). The more-complicated groups that replaced the Yang-Mills group also have only a rather small number of representations, corresponding to the proton and neutron and to the several excited states (other hadrons) that derive from them. Since only certain specific system-states fulfil the group requirements, the groups pertaining to those symmetries are designated as *discrete or non-continuous* groups.

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[6] That is, $\psi \rightarrow \psi'' = e^{i\lambda}\psi$ and $f_p \rightarrow f_p'' = f_p - \partial\lambda/\partial x_p$.

[7] The Lorentz transformations for a body moving with constant velocity (v) in the x direction are: $z'' = z$: $y'' = y$: $x'' = k\,(x - v\,t)$: $t'' = k\,(t - v\,x\,/\,c^2)$, where $k = (1 - v^2/c^2)^{-1/2}$ and c is the velocity of light.

Extensions and modifications of the Yang-Mills proposal (and also subsequent experimental developments) eventually led to the current Standard Model of Particle Physics (Cottingham and Greenwood 2007) which treats hadrons as composed of spin one-half fermions held together by bosons—vector particles of unit spin that arise from quantization of gauge fields (as *the photon*, the boson that carries electromagnetism, arises from quantization of the electromagnetic gauge field).[8] Spatiotemporal symmetries (such as those of spatial rotation) are called external, global, or geometric: Phase-symmetry in electrodynamics and isospin-symmetries are designated internal, local, or dynamic: this usage corresponds to a *major extension* of the concept of symmetry.[9]

The principle that every individual corresponds to a representation of a mathematical group responds to the external (epistemological) part of the composition question: the requirement that operations which combine members of groups *always produce members of the group* answers the internal (ontological) sub-question. Stability is achieved only when relationships internal to each item demonstrate such *closure* that states of the system repeatedly reoccur—so that the system persists through time. This restriction is severe. Section 4 describes several ways in which that restriction may be satisfied.

4 *Varieties of Closure*

4.1 Closure Louis de Broglie

After the First World War Louis de Broglie (1892–1987) resumed his university studies and collaborated with his older brother Maurice, an accomplished physicist. In 1922, the brothers de Broglie confirmed the astonishing report that electrons produced by impact of X-rays on metals had velocities *just as large* as the velocities of the electrons used to generate those X-rays. This was as if throwing a log into a lake should cause one similar log (out of many on the other side of the lake) to jump up *with equal energy* (de Broglie and de Broglie 1922).

At that time, theories of the internal structure of atoms that had been devised by Bohr and by Arnold Sommerfeld could adequately rationalize available data on the line spectra of atomic hydrogen and ionized helium—but only by making the assumption that electrons within atoms are restricted to having *only certain energy-values*. Those early versions of quantum mechanics (QM) *could not explain*: "why, among the infinity of motions which an electron ought to be able to have in the atom according to classical concepts, only certain ones were possible" (de Broglie 1965, 246). Louis de Broglie deduced from Einstein's theory of relativity and early versions of quantum theory that each material object (including electrons within

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[8] The Standard Model does not have a single theoretical basis, but rather is a collection of ad hoc sub-models (MacKinnon 2008).

[9] Eugene Wigner remarked: "The concept of symmetry and invariance has been extended into a new area—an area where its roots are much less close to direct experience and observation than in the classical area of space-time symmetry… (Wigner 1967, 15).

atoms) must have wave-properties. He wrote: "The fundamental idea of the theory of the quantum is the impossibility of depicting an isolated quantity of energy that is not accompanied by a certain frequency" (de Broglie 1972, 1316).

In a 1923 *Comptes rendus* note, Louis de Broglie proposed that each electron had *two* characteristic frequencies, an *intrinsic* frequency associated with its rest-mass, and a second frequency that pertained to a wave that moved in the same direction as the electron. With respect to electrons moving on a closed trajectory, he introduced the following postulate:

> It is *almost necessary* to suppose that the trajectory of the electron will be stable *only if* the hypothetical[10] wave passing O' catches up with the electron in phase with it: the wave of frequency ν and speed c/β has to be in resonance over the length of the trajectory
>
> (DE BROGLIE 1923A, 509).

That is to say, an atomic system would be stable (that atom would persist as a unified entity) *only if* the extrinsic wave remains in phase with the internal vibration of the electron corresponding to its intrinsic frequency. The extrinsic wave was then called the phase wave.

In fulfilling this postulate, each possible arrangement of an atomic system engenders another subsequent state of the system that also fulfills the criterion. This feature insures that the system, as a coherent unit, persists through time. The *only if* in the postulate (emphasized in the original French) identifies a clear requirement that a specific relationship between multiple quantities (phases of two vibrations in this case) must obtain in order for a composite system to be stable. The essential novelty of Louis de Broglie's contribution was to provide *a clear and specific criterion* that served as a basis for understanding why some energy-states of electrons in atoms were capable of persistence while other apparently-equivalent possibilities could not attain such longevity. On the basis of this postulate, Louis de Broglie was able to derive the Bohr-Arnold Sommerfeld criteria for the stable energy-states of the electron in the hydrogen atom. This was a great triumph. In a second 1923 note, he predicted that (material) electron-beams would be diffracted as light-beams are (de Broglie 1923b).

Early in 1927, two groups of experimentalists independently confirmed de Broglie's prediction of electron diffraction—validating a second major achievement for him. On the basis of his 1924 doctoral thesis, Louis de Broglie received the 1929 Nobel Prize for Physics. Through Einstein's mediation, that thesis also had facilitated the 1925 development of Schrödinger's wave equation—from which the many impressive results of quantum mechanics flow. However, even before Stockholm Nobel festivities celebrated de Broglie's award, his realistic but non-local pilot-wave interpretation of QM had been supplanted (Bonk 1994) by the non-realistic but local Copenhagen Interpretation (CI). The main proponents of CI were strongly influenced by anti-realistic philosophical ideas current in postwar (Weimar) Germany (Cushing 1994).

Closure of networks of relationships (*Closure Louis de Broglie*) is necessary for persistence of stable things, including chemical entities. This requirement has not been emphasized in past and current philosophical discussion of how properties cohere, but it does respond to the second (ontological) part of the composition question: How is it that several Xs can constitute a Y? Criteria analogous to the one that de Broglie discovered provide the basis by which each of the possible states of a system produces a subsequent state that has the same characteristics. This suggests that it should be possible to interpret each of those states as a representation of some mathematical group. Similar situations should obtain for every persistent chemical entity.

4.2 Closure Henri Poincaré

Philosophic discussion of composite objects generally assumes that properties of composites depend only ("supervene") on the properties of components (Armstrong 2010, 29–32)—the properties of the least-extensive level are held to determine all properties. Whatever its strengths in other fields may be, this doctrine *does not apply* in chemistry. Chemical entities arise from and are sustained by *interactions* among their constituents —and mainly derive their characteristics from those interactions, rather than from properties of the components.

Characteristics of dilute gases can sometimes be inferred from information regarding component molecules—based on the approximation that each molecule acts independently. However, when gases are cooled correlations of molecular motion develop, first over short ranges then over longer distances. Motions of individual molecules become interrelated—so that the properties of the macroscopic sample *cannot* be inferred by mere addition (or other straightforward combination) of the properties of the component molecules.

Similarly, the simple model that chemical reactions occur by *elementary steps*—events that involve instantaneous collisions of pairs of molecules—seldom is even approximately correct. Generally, in reactions of gaseous species "sticky" collisions produce *resonances* (transient aggregates) and give rise to *correlations* among the properties of molecules. Reactions in condensed media (e.g., fluid solutions) are even more subject to cooperative influences than gas-phase reactions are.

In both cool-gas and chemical-reaction cases, as correlation increases application of fundamental theory rapidly becomes unwieldy and impracticable. At certain parameter-values (singularities) computations become *impossible in principle*—as computed quantities go to infinity. In the late nineteenth century, while dealing the motions of the planets in the solar system, Henri Poincaré (1854–1912) encountered situations in which standard methods of physical mechanics failed due to the presence of singularities. In such cases, when near singularities, he replaced variables with divergent series (*asymptotic expansions*). This technique (Berry 1994) allowed otherwise intractable problems to be handled—but it had unexpected consequences. Often, after the variable-replacement, the equations that best described the situation *changed discontinuously* at the

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[10] This replaces "fictional" as a translation of the French "*fictive*."

singularity. Poincaré found that beyond the singularity relatively simple expressions—that emphasized contextually important features and suppressed irrelevant detail—often applied. Similar situations occur in electrodynamics. Interaction of the charge of the electron with the vacuum complicates computation of the charge and mass of the electron from experimental data (Teller 1988)—but renormalization (a procedure related to the asymptotic expansion method that Poincaré devised) makes a self-consistent theory of electrodynamics possible. Similar approaches facilitated adequate understanding of solid-liquid-gas phase changes, critical behavior for pure substances, and transitions between ferromagnetic and paramagnetic behavior (Batterman 2011): analogous techniques are also used in molecular-dynamics-based approaches to chemical reaction kinetics (Jaffé, Kawai, Palacián, Yanguas, and Uzer. 2005, 194).

The simpler description that asymptotic expansion yields at and after singularities typically has different semantics (another *topology*) than the fundamental-level description that applied before the singularity. Properties of correlated systems *do not supervene* on properties of components—they require quite new and topologically-incommensurable descriptions (Atmanspacher, Amannn, and Müller-Herold 1999; Batterman 2011; Bishop 2012; Bishop and Atmanspacher 2006; Primas 1998, 2000).

When cooperative interaction of units becomes dominant, situations adequately described by fundamental theories change into situations that require approaches that use quite different sets of entities, and other kinds of relationships among entities than are used in the fundamental theories. Transition between these diverse *topologies of explanation* may properly be regarded as *a second kind* of closure (*Closure Henri Poincaré*). Like Closure Louis de Broglie discussed in the previous section, Closure Henri Poincaré vitiates assumptions that properties of entities can adequately be understood on the basis of descriptions based on properties of component parts. That sort of closure also underlies the persistence and effectiveness of higher-level entities that result from lower-level cooperativity.

This situation is well described by Hans Primas: "The task of higher-level theory is not to approximate the fundamental theory but to represent new patterns of reality" (Primas 1998). Physics Nobel laureate Robert Laughlin argued (2005) that aspects of fundamental physics *result from* cooperative interactions.

4.3 Closure Ilya Prigogine

Investigation of the properties of networks of processes (such as interconnected chemical or biochemical reactions) is an active field of twenty-first-century science. Such studies show that *modes of dynamic closure* determine the coherence of properties of important systems, including flames, hurricanes, biological organisms, ecologies, and human societies. Chemical systems conveniently clarify fundamental principles of such coherences.

Networks of chemical processes operating in far-from-equilibrium conditions often give rise to *oscillation* of concentration of components. If the system is *closed*, such repeated concentration-variation eventually dies out. However if the system is *open*, so that reactants can continuously enter and products exit, then oscillations may continue indefinitely. In stirred systems, chemical oscillations may be either gradual or sharp: In the latter case, immense numbers of chemical ions or molecules undergo coordinated chemical change in a fraction of a second. Such dynamic chemical coherences necessarily degrade chemical energy and increase *entropy* (overall disorder). This type of organization is called dissipative structure. Chemists—particularly Belgian physical chemist Ilya Prigogine (1917–2003, Nobel Prize in Chemistry 1997)—have made major contributions to our understanding of such coherent organization of processes in far-from-equilibrium open systems (Prigogine 1977, Kondepudi and Prigogine 1998, Earley 2012a, Lombardi 2012).

Each chemical dissipative structure involves a reaction (or set of reactions) that *gets faster as it goes on*—an autocatalytic process. The simplest example is $A + B \rightarrow 2B$ (where the rate of reaction is proportional to the product of concentrations of A and of B). In this case, B is a *direct autocatalyst*. Many kinds of interaction that facilitate coordinated or cooperative functioning produce *indirect* autocatalysis (e.g., Sugihara and Yao 2009). Systems that involve direct or indirect autocatalysis tend to be *unstable*—they readily explode and disperse. However, if such a system also involves one or more processes that *suitably reduce* the autocatalysis (such as $B + C \rightarrow D$) then the system may return to its original condition, and even do so repeatedly, thereby generating *continuing oscillations*—a type of long-term persistence (Earley 2003a).

When oscillations occur in open-system chemical systems, variations of concentrations of several components can be followed often over long time periods. Careful study of such *time-series* (along with relationships among times-series for diverse components, and responses of the system to perturbations) yields information on the details of the chemical reactions underlying the continuous oscillations. When concentrations of system-components vary in a *correlated* way, the variation of one may cause the change in another, or alternatively, both may independently depend on some third factor. Studies of relationships among time-series may discriminate between such possibilities if the system is followed for sufficiently long times (Sugihara, May, Ye, Hsieh, Deyle, Fogarty, and Munch 2012). In many cases, explicit mathematical models of chemical mechanisms reproduce main features of observed time-series (and/or illustrate important behaviors of dynamic coherences).

In each such open-system dynamic coherence, the rate of entropy-generation in the presence of the coherence is greater than it would be in the absence of the coherence-defining closure. Also, the effects of the coherence on other items are *quite different* from effects of the same components but without the closure. Therefore the system *as a whole* makes a difference. That coherence must be counted as one of the items that comprise the world (Ney 2009, Earley 2006)—that is, the dissipative structure *as a whole* has *ontological* significance. The effects of the structure are the sums of the effects of the components, but *which components persist* in the system depends on the details of the closure of the network of reactions. The *closed network* of relationships regulates the *composition* of the system. For example, the existence of biological dissipative structures accounts for the production (and therefore the existence) of high-energy molecular species such as sugars, proteins, and DNAs, but those molecules are themselves components of the dissipative structures that produce them. Components are influenced by the characteristics of the coherences which those same components constitute.

Networks of non-linear chemical processes share important characteristics with other complex dynamic coherences, including biochemical oscillations, cardiac rhythms, ecological developmental changes, and financial-market variations. *Closure of networks of processes* is essential for all such persistent dynamic coherences. We designate this as *Closure Ilya Prigogine.*

4.4 Robustness of Biochemical Dissipative Structures

Surprisingly, some chemical species that are involved in networks of biochemical reactions somehow remain at quite constant concentrations for long periods. This *robustness* of concentration occurs both in vitro and in vivo, and can be modeled in silico. Robustness in a network facilitates incorporation of that coherent set of relationships as a reliable component part of more-inclusive dynamic systems. A remarkable theorem (Shinar and Feinberg 2010) clarifies what network characteristics are needed to generate the approximate concentration-robustness that is experimentally observed. Specific network properties provide necessary and sufficient conditions for insuring long-term stability of some concentrations.

Robustness, considered the ability to continue to function in spite of both internal and external fluctuations, occurs at an amazing variety of nested biological levels. Each of the following illustrations of robustness is well documented (Wagner 2005): The sequence of codons in RNA and DNA is insensitive to replication errors; the function of proteins does not depend on point-mutations in codons; RNA secondary structure is immune to changes in nucleotides; the spatial structure and function of proteins does not depend on the amino acid sequence of the protein; the expression function of a gene is robust to mutations in regulatory regions; the outputs of metabolic pathways are little influenced by changes in regulatory genes; genetic networks function even when interactions among network genes alter; metabolic-network function is not sensitive to elimination of specific chemical reactions from the network; development of phenotypic patterns persists even though component genes vary; body-plans of organism survive modifications in embryonic development. Each of these achievements of robustness involves closures that are themselves intricate combinations of simpler sorts of closure.

4.5 Closure Jacques Cauvin

Propensity to engage in cooperative interactions is arguably the most salient characteristic of *human* individuals. Many of the features of the various worlds we all inhabit are institutional facts—objective realities that are held in being

by their widespread acceptance (Searle 2010). Human institutions (e.g., specific languages and ways of living, as well as economic, political, and religious systems) are all based on (usually unconscious) human cooperativity. In all such cases, relationships among constituents must themselves be so interrelated that coherences maintain definition and identity over time. In these cases, system properties do not supervene on properties of constituents. Anthropologist Jacques Cauvin (2000) explored how *prior changes* in concepts and social practices *made possible* initial development of agriculture, and thereby grounded the flourishing of subsequent human cultures. We designate any mode of interrelation of processes which makes *further network-formation* possible as *Closure Jacques Cauvin.*

Marjorie Grene (1978, 17) observed: "We do not just *have* rationality or language or symbol systems as our portable property. We *come to ourselves* within symbol systems. They have us as much as we have them." Cauvin's insight has been developed by recent studies based on evolutionary network theory (Atran and Henrich 2010; Richerson, Boyd, and Henrich 2010) that have clarified how human agents are themselves shaped by relational networks—at the same time are each of those networks has been created by the behaviors of such agents.

Louis de Broglie clarified (for his time) how coherence of electrons and protons *constitutes* atoms. Henri Poincaré demonstrated how *new kinds of relationship* (novel topologies) result from cooperative interactions. Ilya Prigogine clarified how far-from-equilibrium dynamic coherences persist in open systems such as when interactions generate large-scale coherences. Jacques Cauvin showed how *conceptual innovations* (influential institutional facts) made possible the distinctive evolution of *human* societies. In each of these diverse cases, the emergence of novel modes of effective functioning (*properties*) depends on defining *closures of relationships* of components. There surely are other significant modes of closure. *Closure* provides the basis for the origin of novel centers of influence—and thereby grounds the *ontological* changes which are brought about by cooperative interaction.

5 *Structures and Properties*

5.1 The Structuralist Revival

Considerable attention has recently shifted to *structuralist* philosophical approaches to scientific (especially microphysical) questions (e.g., Bokulich and Bokulich 2011, Landry and Rickles 2012).[11] In 1989 John Worrall pointed out that although entities postulated by scientific theories do change over time, *structural* aspects of theories tend to persist through such *ontological* modifications. He proposed that what we learn in scientific investigation is correct, but that we learn only about structures—not about entities. This approach, called

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[11] Such approaches were widely discussed in the first third of the twentieth century (e.g., Eddington 1935).

Epistemological Structural Realism (ESR) claims that *relationships* are more important than are the *entities* that are related. Others carried this reasoning further and concluded that structure is not only *all that we can know* but also that structure is *all that exists* to be known. Steven French (in French and Ladyman 2011, 30), for instance, "dispenses with objects entirely." This more-radical view is called Ontological Structural Realism (OSR). However, the notion of structures of relationship which do not involve items that are related ("relations without relata") seems paradoxical.

Earlier suggestions of the philosophic importance of structures had specifically focused on chemical problems. David Armstrong (1978, *Vol. 2*, 68–71) recommended that "being a methane molecule" should be considered to involve a structural universal (a multiply realizable polyadic relationship that necessarily involves "being carbon," "being hydrogen," and "being chemically bonded" as correlative universals).

5.2 Are Any Properties Intrinsic?

Some versions of OSR consider that *all* properties of any entity are *structural* properties—characteristics that depend on relationships with other entities within structures. This amounts to a denial that entities have *intrinsic* properties—characteristics that they would possess if fully isolated so as to be independent of all relationships. Two recent moderate versions of OSR provide for intrinsic properties as well as relational ones—and (their adherents claim) thus resolve the relationship-without-relata conundrum and introduce causal necessity (modality) into structural realism (SR).

In one such proposal, Holger Lyre agrees that all properties are structural, but holds that some structural properties are "structurally derived intrinsic properties (invariants of structure)" (Lyre 2010, sec. 6). He had previously considered the relationship between OSR and the symmetry-group (U(1)) which applies to electromagnetism and concluded that, in permutable theories,[12] description of objects as solely group-theoretically constituted "becomes mandatory. For there we only have access to the objects as members of equivalence-classes, under those symmetry transformations which leave the physical properties invariant" (Lyre 2004, 663). In order to establish that some structural properties are intrinsic, Lyre points out: "An object may have its invariant properties according to the world's structure: the structure comes equipped with such properties" (Lyre 2012, 170). Perhaps to allay suspicion that he might be advocating *ante rem* Platonism, he insists: "The world structure must... be an instantiated structure" (Lyre 2012, 170).

In an alternative proposal designed to introduce causal necessity into SR, Michael Esfeld advocates Causal Realism (CR). He initially proposed that all properties are *causal properties* (powers[13]) and rejected the (characteristically Humean) doctrine that some properties are *categorial*—merely qualitative with no relation to causality (Esfeld 2003). Subsequently, he conceded: "we no longer take OSR—at least in the moderate version that we defend, recognizing objects—to be opposed to the acknowledgement of the existence of intrinsic properties, as long as such intrinsic properties do not amount to an intrinsic identity of the objects" (Esfeld and Lam 2011, 155). He claims that structures (as well as properties) must be causally efficacious:

> Structures can be causally efficacious in the same sense as intrinsic properties of events: as events can bring about effects in virtue of having certain intrinsic properties, they can bring about effects in virtue of standing in certain relations with each other so that it is the network of relations—that is, the structure as a whole—that is causally efficacious.
>
> (ESFELD 2012, sec. 3)

He further claims that: "In sum, ontic structural realism is suitable as a form of scientific realism only if it commits itself to causal structure, that is to say, only if the essence of the fundamental physical structures is taken to consist in the power to produce certain effects" (Esfeld 2009, 188).

5.3 Can Structures Be Causes?

There are objections to the entire structural-realist project. F. A. Müller claims that proponents of structural realisms do not adequately specify the meaning of structure—and that the two best-established formal definitions of structure do not have the properties that structural realists require. He claims: "neither set-theoretical nor category-theoretical notions of structure serve the needs of structural realism" (Müller 2010, 399). Stathis Psillos, a persistent critic of SR, argues that OSR incoherently requires that structures be both *abstract* (multiply realizable) and *concrete* (causally efficacious)—but since structures (considered as polyadic properties) are *purely mathematical* entities they cannot have *causal* efficacy—and therefore structures do not have modal force (Psillos 2012).

Rom Harré and E. H. Madden (1975) revived the moribund notion of causal powers, but Harré (2002) urged members of the Critical Realist school of social psychology (an approach based on Harré's prior work) to cease ascribing causal power to impotent fictions such as "the banking system." Subsequently Harré (2009b) identified the tendency toward reification ("substantialism") as lying at the root of the errors he decried—and even went so far as to assert: "Structural models in the human sciences are heuristic models only—there are no structures" (Harré 2009a, 138). This Neo-Thacherian dictum appears to contrast strongly with some of Harré's earlier statements, specifically: "Structured groups, that is, collectives, are ontologically prior to individuals.

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[12] Those which concern particles (such as protons) which cannot be distinguished from other particles of the same sort.

[13] George Molnar (2003, 60–81) tried to account for "how these properties [powers] have an object toward which they are oriented or directed" and postulated *physical intentionality*, but did not give a convincing account of it.

Human beings are constituted as people by their interpersonal relations" (Harré 1993, 34), and: "Forms of life are the contexts in which personal and social identities are formed" (Harré 2009a, 142).

In his discussion of social causation Harré identified two modes of causal action—*event* causality and *agent* causality. In event causality some happening activates a mechanism that engenders a subsequent result; in agent causality some *continuously existing and active being* brings about consequences without external stimulation (save, perhaps, removal of obstructions). Harré proposed that detection of event causality requires identification of a *mechanism* that connects an initiating occurrence with an ensuing result: Recognition of agent causality demands location of one or more specific *powerful particulars* that act continuously (unless that action is somehow blocked). Harré concluded that only *individual human persons* qualify as causal agents in social psychology—vague constructs such as the banking system certainly do not merit that designation. Both of the modes of causality Harré identifies involve powerful particulars (either events or continuants); neither of them implicates universals (properties, relations, or structures) in causality. If, as Esfeld claims, the validity of OSR depends on structures having causal power, then structuralists need to respond to the objections of Müller, Psillos, and Harré by clarifying how (or in what sense) structures may properly be considered causes.

6 *Causes and Determinants*

6.1 Concepts of Causation

The word *cause* has several distinct meanings in standard English—it is polysemic. *The Shorter Oxford English Dictionary* (SOED) identifies *four* connotations of cause corresponding to: (1) agent, (2) reason, (3) lawsuit, and (4) social movement. Chemists use cause to refer to both agents and reasons. In contrast, philosophers generally recognize only the first (agent) meaning of cause given in the SOED, and regard all other uses as suspect—or just wrong.

Ernan McMullin (1999) quoted the section of Aristotle's *Physics* (194b, 18–20) that introduces the four types of cause (material, formal, efficient, and final)—"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)." This definition appears to identify cause and reason. McMullin concluded that what Aristotle meant by *cause* differs in important ways from how most philosophers now understand that term.

Although Aristotle counted any adequate response to a why-question as a cause (*aitiā*), he also made a clear distinction between *efficient* causes (change-initiating agents) and *formal* causes—arrangements necessary for an event to occur. As Psillos (2012) points out, structures are formal: The objection that structures *cannot be* causes seems related to the distinction between efficient and formal causality. Robert Pasnau (2004) carefully described how, during the rapid development and subsequent slow decline of medieval Scholastic Philosophy, the understanding of the Aristotelian concept of substantial form (roughly equivalent to the modern notion of structure) gradually changed away from its original (purely formal) Aristotelian meaning, and increasingly acquired overtones of efficient agency. Pasnau concluded that the further modifications in the usual philosophical understanding of cause which subsequently occurred should be interpreted as continuations of that trend.

With the success of Newtonian physics, only interactions similar to events on billiard tables (where precisely determined impacts yielded exactly predictable results) came to be considered as causally significant interactions. *Impact* of impenetrable corpuscles became the paradigmatic causal process; *efficient* causality took over the designation cause. Most philosophers relegated any other factors that might be involved in answers to why-questions to subordinate status—or to oblivion.

6.2 Limits to Agency

Mario Bunge pointed out that:

> Some of the grounds for the Renaissance reduction of causes to the *causa effciens* were the following: (a) it [the efficient cause] was, of all the four [Aristotelian causes], the sole clearly conceived one; (b) hence it was mathematically expressible; (c) it could be assigned an empirical correlate, namely an event (usually a motion) producing another event (usually another motion) in accordance with fixed rules...; (d) as a consequence, the efficient cause was controllable; moreover its control was regarded as leading to the harnessing of nature.
>
> (BUNGE 1959, 32)

However, although Bunge does "restrict the meaning of the term cause to *efficient cause*, or extrinsic motive agent, or external influence producing change" (33), he also recognizes that "causation... is only one among several types of determination; there are other types of lawful production, other levels of interconnection" (30). He distinguishes between *causes* (effective agents—the *how* of things) and *reasons* (rational explanations—the *why* of things), pointing out that these two notions are often confounded: "The identity of explanation with the disclosing of causes is even rooted in the Greek language, in which *aition* and *logos* are almost interchangeable since both mean cause and reason. The confusion of cause with reason, and that of effect with consequent, are, moreover, common in our everyday speech" (226–227).[14]

Biologist Ernst Mayr—a founder of the modern synthesis in evolutionary theory—urged (1961) that biologists clearly distinguish proximate causes from ultimate causes. The *ultimate causes* of the long-distance migrations of certain birds, for instance, are (in Mayr's view) the historical explanations (largely in terms of natural selection) that account for *why* those birds carry out such journeys: the *proximate causes* are whatever hormonal changes (or other internal

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[14] Bunge subsequently observed: "From the point of view of cognitive neuroscience, reasons for acting are efficient causes" (Bunge 2010, 224).

mechanisms) account for *how* that behavior-pattern works out in practice. In Bunge's terminology, Mayr's ultimate causes are not causes but reasons; only Mayr's proximate causes would properly be designated causes (as current philosophers use that word).

It is now clear that most interesting biological systems do not fit Mayr's recommendation nearly as well as seasonal bird migrations do. Avian flight patterns have vanishingly small effects on the progression of the seasons—cause and effect are quite distinct—but, in contrast, the vast majority of biological systems involve *reciprocal* (rather than *unidirectional*) causality, so that Mayr's distinction does not apply. In discussion of this point, Kevin Laland and his colleagues report: "When a trait evolves through intersexual selection, the source of selection is itself an evolving character. The peacock's tail evolves through though the mating-preferences in peahens and those preferences coevolve with the male trait" (Laland, Sterelny, Odling-Smee, Hoppitt, and Tuler 2011, 1512). Whenever *reciprocal determination* makes it impossible cleanly to distinguish causes from reasons, restricting causality to *efficient* causes (as philosophers recommend) is not appropriate.

6.3 Peircean Determinants

T. L. Short (2007, 105–107) observed that the narrowness of the contemporary philosophic understanding of causation (a baleful influence, he says, of Hume's ghost) has unfortunate effects—but called attention to an understanding of causality developed by Charles S. Peirce. Stephen Pratten (2009) suggested that Short's interpretation of Peirce's causal theory provided an adequate response to Harré's conclusion that structures cannot be causes.

The interactions that classical mechanics deals with have time-reversal symmetry: Videos of billiard-ball collisions look the same whether running forward or backward. In contrast, many natural processes *proceed in only one direction.* (The spark-induced explosion of a mixture of H_2 and O_2 loudly leads to rapid production of H_2O: the reverse reaction is unobservable.) Peirce calls such unidirectional processes "finious;" Short suggests the designation "anisotropic;" chemists call such changes "irreversible." Pierce held an alternate kind of causal process obtains in irreversible processes—"that mode of bringing facts about according to which a general description of result is made to come about, quite irrespective of any compulsion for it to come about in this or that particular way; although the means may be adapted to the end" (CP 1.211). This corresponds to understanding cause as reason rather than as agent—that is, to using the second denotation of the English word cause given in the SOED, rather than the first.

Peirce considered that Darwin's account of the origin of biological species exemplifies this alternative mode of result-determination. Natural selection gradually (and irreversibly) eliminates those characteristics of organisms that are not suited to the environmental conditions that prevail. Such reduction (culling) of possibilities eventually produces one particular determinate result—which outcome is produced depends on the contingencies of the culling rather than on the action of underlying agents.

> There remains little doubt that the Darwinian theory indicates a real cause, which tends to adapt animal and vegetable forms to their environment. A very remarkable feature of it is that it shows how merely fortuitous variations of individuals together with merely fortuitous mishaps to them would, under the action of heredity, result, not in mere irregularity, nor even in a statistical constancy, but in continual and indefinite progress toward a better adaptation of means to ends.
> (CP 7.395)

Natural selection works in such a way as to produce adaptation of life-forms to their circumstances (Thompson 2012). This general aim "does not determine in what particular way it is to be brought about, but only that the result shall have a certain general character. The general result may be brought about at one time in one way, and at another time in another way" (CP 1.211).

On this basis, Peirce considers that each effective selection-criterion is a *general* rather than a *particular* (a universal rather than a substance). Each such criterion might be called a *controlling general*—an outcome-determining universal. By this means structures (closures of relationships that have the property of engendering future versions of the same closures) would have result-shaping effects, although they are not agents. In other words, if a certain state-of-affairs results from a *prior selection* on the basis of some criterion, that criterion (a universal) is a determinant (a cause in a general sense) of that state of affairs. To the extent that closure of a network of relationships of components is a prerequisite for the stability of entities, that closure (which corresponds to a structural universal) is also a *necessary determinant* of the states of affairs that it engenders. The key feature is that if an *equivalent to selection* accounts of the existence of a structure, then the influence of that structure (as such) may properly be termed a determinant—a cause, in a sense that is more general is usually recognized by the dialect of the province of the philosophers.

6.4 Non-Agentive Determination in Oseltamivir-Resistant Swine Flu

Several experimental results have recently been reported that show how *structural* features *determine outcomes* as reasons rather than as agents.

Since 1990, millions of people have been sickened by swine flu—infection by the H1N1 influenza virus. From its introduction in 1999 until recently the drug oseltamivir (Tamiflu, Hoffman-LaRoche) has been effective against swine flu. However, during drug-testing, a mutation (named H274Y)[15] made the virus immune to oseltamivir—but also impaired infectivity of the virus and *did not reduce* the drug's effectiveness. In 2007 several oseltamivir-resistant strains of the virus with *no reduction in virulence* appeared. Bloom, Gong, and Baltimore (2010) found that two additional mutations[16] had occurred independently and enabled the virus to tolerate subsequent H274Y mutation without loss of virulence. The first new mutation was ineffective: the second mutation increased

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[15] Tyrosine (Y) replaced histidine (H) at position 274 in the virus DNA.

[16] L111Q and S106P.

the effectiveness of the otherwise-innocuous first mutation: *combination* of the mutations was result-determining. Such a combination (as a determinant of the outcome) is not an *efficient* cause. It is a *reason* not an *agent*. Determinants of this sort can be identified when some arrangements function while others fail. Such pruning defines a result.

Tenaillon, Rodríguez-Verdugo, Gaut, McDonald, Bennett, Long, and Gaut (2012) and Meyer, Dobias, Weitz, Barrick, Quick, and Lenski (2012) reported other examples of non-agential determination. In each case a result depended on actions of particulars but those actions *did not determine* the result: *Selection constraints* specified the outcome. Rather than actions of components determining the outcome, constraints determined *which* components acted—and thereby specified what actually happened.

6.5 Contextual Determination

Every macroscopic state of affairs involves myriads of microscopic and submicroscopic components. In the absence of external constraints (so all components are independent) each sample would have an immense number of equally-probable possible future states. *But no real system is unconstrained.* Every sample has a history (usually unknown and untold) that specifies its current context and limits the range of available futures (Earley 2012b). Theories that apply at the level of micro-components provide *necessary conditions* for properties of more-inclusive coherences—but they *do not provide sufficient conditions*: Sufficient conditions must be dealt with by less-fundamental approaches. An open vat of nutritious broth quickly changes into a teeming mass of biological organisms, but *which specific type(s)* of organism result depends on the particular species that happen(s) happily to colonize that soup.

"There are properties of the higher-level theories (chemistry and thermodynamics) for which the full arsenal of the fundamental theories (quantum mechanics and statistical mechanics) provide no sufficient conditions for their derivation or definition" (Bishop and Atmanspacher 2006, 1755). By *contextual property emergence*, upper-level properties derive from the *context of constraints* of the system as well as from the underlying level which involves less-extensive components. Upper-level constraints typically remove degeneracies that characterize lower-level situations and thus lead to *stable* states. "Necessary conditions due to the original topology of the basic description are not violated as the new topology is consistent with (though not implied by) the original topology." Such constraints are *contextual determinants*.

The network of relationships that underlies and defines an emergent coherence corresponds to one or more *structural universals*. The problem of the modality of structural realism arises from the concern that mathematical objects (such as structural universals) should not directly have physical effects. In the cases considered here each structural universal corresponds to the closure of a network of relationships—a physical process that has consequences. Closure of networks of interactions among components generally leads to situations that persist and/or recur. This is how behavior-patterns (properties in Peirce's sense) of substances remain coherently related over time.

6.6 Ordinary Things

But what about ordinary entities, such as David Robb's tennis ball Alpha (discussed in section 1.6, above)? How can we understand the coherence of Alpha's properties? That tennis ball coheres and behaves as a unit because the many billions of elemental centers (atoms) that make up that sphere adhere to each other through rather stable chemical bonds—each one a closure of attractive and repulsive forces that is protected from disruption by activation-barriers. But why do those particular bonds exist rather than others? Why is Alpha small and yellow rather than some other size and color?

The International Tennis Federation (ITF) defined the official diameter of a regulation tennis ball as 65.41–68.58 mm (2.575–2.700 inches), and ruled that balls must weigh between 56.0 g and 59.4 g (1.975–2.095 ounces). Yellow and white are the only tennis-ball colors that are approved by the United States Tennis Association (USTA) and the ITF. Since 1972 most tennis balls have been made in a specific fluorescent yellow color—because research showed that balls of that color were more visible on television that those of any other color. The properties of tennis ball Alpha depend on the well-understood physical and chemical factors that determine how chemical bonds relate to each other—but also on contingent historical, economic, and psychological factors that influence decisions of the USTA and ITF committees that specified what properties are necessary for a ball to qualify as a regulation tennis ball. In this sense Alpha is as much an evolved system (in Wimsatt's trichotomy) as is any biological species or individual. Production of tennis balls (what Peirce would have called a *finious* process) is clearly much influenced by determinants of several types, whether or not philosophers would designate such factors as causes.

In Robb's example, and in all other cases, closures of relationships of constituents—determining structural universals—serve as *criteria for selection* among results of activities of powerful particulars. In each case, coherence at any level influences and depends on both wider and narrower (more-inclusive and less-inclusive) integrations. The characteristics of material objects that philosophers discuss depend on closures that involve chemical components—and also on human decisions within more-or-less stable cultural integrations (institutional facts).

Properties stay together in each chemical entity because networks of dynamic relationships among components generate a *closed* set of subsequent states. Each such closure depends on continuance of closures in its components, and also may participate in (and be determined by) closures of more-inclusive relationship-networks. Structures (polyadic relationships) *determine* specific outcomes, even though they are not themselves *agents*.

Throughout human evolution people have modified naturally occurring materials to produce useful items. Major cultural advances occurred when chemical processes (cooking, baking of ceramics, ore-smelting, etc.) were first used to *improve* natural resources. Arguably tin-bronze was the first artificial material *intentionally synthesized* in order to produce *specific properties* important for more-inclusive coherences. In the third millennium BC, techniques for manufacture and use of effective *bronze daggers* spread (remarkably rapidly) throughout lands surrounding the Aegean Sea: "Just as every nation in the Levant need[ed] tanks in the 1960s and 1970s, so every man needed a dagger during the bronze age" (Renfrew 2011, 320).

In our own culture, most of the items with which we deal are made of artificial materials. From one point of view, behavioral characteristics of each such item hang together because of chemical bonding: in a another sense, those properties exist because each item is *useful in some context*—and that *criterion of utility* motivated the designer, manufacturer and purchaser. On that basis, every artifact which contains artificial materials is *an evolved system* in Wimsatt's trichotomy. Diachronic modes of thought must be used to understand all items: *synchronic* methods—attempting to understand coherences in terms of their current composition without attention to how those integrations came to be—yield wrong conclusions.

Persistence of every entity depends on *closure* of relationships among its components (each part must be stable enough) and is also determined by higher-level integrations of which that entity is a component. Creative activity, some involving human action, continually generates "new shapes of value which merge into higher attainments of things beyond themselves" (Whitehead 1967, 94).

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