Modes of *Chemical* Becoming

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Abstract: In the characterization of the $ArCl_2$ 'van der Waals complex', a recognizable pattern of well-defined peaks is observed in the microwave absorption spectrum. In the control of chaos in a chemical oscillatory reaction the power spectrum progressively becomes simpler, at length yielding a single peak. Since both of these cases generate coherences that are centers of agency, they should be considered to produce new chemical entities. Applicability of this ontological approach to coherences of wider societal interest is suggested.

Keywords: *ontology, chemical entities, van der Waals complexes, chaos, coherence, oscillatory reactions.*

I. Introduction: Ontological Approaches to Chemical Change

Historically, important philosophical discussions of becoming (including those of Aristotle, Kant, Hegel, and Peirce) considered phenomena and entities that are now squarely in the province of chemistry. Chemists are interested in wholes and parts, in connections between features of components and properties of composite entities made up by those pieces. Questions considered by Aristotle in *On Generation and Corruption*, and more-recently discussed by Paul Bogaard (1979) and Mary Gill (1989), are, or ought to be, of interest to both groups of scholars.

Richard Schlagel (1992) has noted that philosophers often treat problems as insoluble for decades (even centuries) after scientists consider them resolved. A 1988 philosophic study titled *Substance and Modern Science* (Connell 1988), notes that during chemical reaction, properties of reactants (gray sodium metal and green gaseous dichlorine, say) are replaced by a quite different set of properties characteristic of the product(s) (brittle, white, sodium chloride). The author then states:

> So given that changes have occurred in almost all the properties, we know that something more than a mere uniting must occur, even though the nature of

HYLE – An International Journal for the Philosophy of Chemistry, Vol. 4 (1998), 105-115.

> the additional activities or interactions is left in the dark. That some sort of interaction must occur cannot be doubted, if observation is to mean anything, but *precisely what the character of the interaction is we have no way of determining.* [Emphasis in original]

It is simply not the case that we have no way of determining what is going on during the becoming of new chemical substances. Contemporary chemists have developed elegant methods to probe intimate details of interactions that go on in the course of chemical reactions. The obscurity suggested in the quotation *does not* exist

A further fairly common misconception is the opinion that the present state of physical science requires (or strongly suggests) that "the final real things of which the world is made up" (Whitehead 1978) are submicroscopic. If one restricts attention to the topics covered in introductory chemistry courses, one might be justified in holding (with Richard Connell 1988) that science considers that: everything is made up of elementary particles, and those particles are 'substances'.

In an extreme version of this doctrine, Peter van Inwagen (1990) holds that nonliving existents are all "simple". He maintains that there are no chairs, just "simples arranged chairwise", and that there is no Sun, just "simples arranged sidereally". If one were to look at presently-active research areas in experimental science, one might reach conclusions quite differently from the notions just mentioned. The ontology, cosmology, and metaphysics implied by much truly contemporary science are quite different from what many philosophers may suppose it to be.

Some authors have proposed metaphysical approaches that are more congenial. In *The Nature of Physical Existence* (1972), Ivor Leclerc proposed an ontology that has both Whiteheadian and Aristotelian features. Leclerc emphasized the requirement (mentioned by Aristotle) that the influences of components of a compound individual on each other be "fully reciprocal". In *The Recovery of the Measure* (1989), Robert Neville proposed a philosophy of nature based on the concept that "all determinate things are harmonies of essential and conditional features".

This paper considers two examples of *chemical becoming* in areas of active, current, experimental, research: 1) 'van der Waals molecules' and 2) transition from chaos to coherent behavior in open chemical systems far from equilibrium. The kinds of chemical becoming discussed here may be interpreted to exemplify what a "harmony of features" (Neville 1989) or "fully reciprocal acting" (Leclerc 1972) might mean, and to extend classical ontology in interesting, and perhaps useful, ways (Earley 1991).

II. The Becoming of van der Waals Complexes: Existence as Power

Experimental and theoretical study of van der Waals complexes made by reactions like:

$$Ar + Cl_2 \rightarrow ArCl_2$$

was a 'hot topic' in the *Journal of Chemical Physics* recently (*e.g.*, Beneventi *et al.* 1993, Xu *et al.* 1993). As you know, argon is a *noble gas*. Argon atoms are not much given to chemical reactivity. Part of the interest of complexes like $ArCl_2$ is their *implausibility,* on the basis of intuitions based on normal chemical experience. A typical experiment in this field is described in the *Journal of Chemical Physics* (Xu *et al*. 1993) as follows:

> The $Ar\text{-}Cl_2$ complex was formed by the expansion of a gas mixture consisting of 0.4% Cl_2 and 0.8% Ar in Ne at a backing pressure of 5.0 atm. It was injected into a[n evacuated] cell with a […] nozzle (orifice diameter of 0.8 mm) mounted in one of the cavity mirrors [of a microwave spectrometer]. The beam ran parallel to the direction of microwave [energy] propagation.

On the basis of the results of their experiments, the investigators concluded that $ArCl_2$ molecules are present in the gas stream, and furthermore that this three-atom species is T-shaped, rather than linear (in contrast, Ar-Cl-F is found to be linear). How are these conclusions reached? It is important to understand this, to clarify the meaning of terms such as 'substance', 'process', 'becoming', and 'existence' among chemists.

The criterion of existence used by the investigators in this case is that the $ArCl_2$ aggregate, as a unified whole, causes observable effects that are not ascribable to any of the components. In *The Sophist (246-247)* – a late work (Hamilton & Cairns, 1961) – Plato discussed a "sort of war of giants and gods" then going on, between "those who make being to consist in ideas […] they are civil people enough" and those "who define being and body as one […] and terrible fellows they are". He proposes an approach different from that of either of the two factions mentioned.

> My suggestion would be that anything that possesses any sort of power to affect another, or to be affected by another even for a moment, however trifling the cause and however slight the effect, has real existence; and I hold that the definition of being is simply power.

This ancient notion is the basis for the criterion of existence generally used by chemists. (Aristotle mentions a similar criterion of existence, but seems not fully to endorse it; *On Generation and Corruption* 318b 24-27.)

III. Characterizing Short-lived Entities

Microwaves are low energy radio-waves used in radar. In the experiment described above, such waves pass through a stream of rapidly-flowing gas containing both argon (Ar) atoms and dichlorine (Cl_2) molecules mixed with a number of helium (He) atoms much (200 times) larger than the number of argon or dichlorine particles. During the experiment, the amount of microwave energy that falls on a detector (after having passed through the gas-stream) is carefully measured, while the frequency of the radiation is gradually changed. If helium alone, or argon in helium, or dichlorine in helium, is passed through the apparatus, *no microwave energy is absorbed*. This is completely understandable, since absorption of this kind of energy by a molecule requires that the molecule have an *un*symmetrical distribution of electrical charge and all of these three molecules (Ar, He, Cl_2) are fully symmetrical. (That is to say, the center of positive charge for each molecule exactly coincides with the center of negative charge for the same molecule.) Ar, He and Cl_2 all *have dipole moments of exactly zero*.

If *both* argon and dichlorine are present simultaneously in the (mainly helium) gas stream, then the gas stream *absorbs some of the microwave energy* passing through it. A display of energy absorbed versus frequency (an absorption spectrum), shows a number of narrow lines. Only radiation with certain *specific* values of energy is picked up by the gas. The microwave energy-range is known to be the range corresponding to *rotation of molecules* for which the center of negative charge does not coincide with the center of positive charge. Energy is absorbed when a molecule is ‘excited’ from one (specific) state of rotational motion to another, higher-energy state. The reason that lines are observed in the microwave absorption spectrum of Ar/He/Cl_2 mixtures can be assigned, with a high degree of confidence, to the existence of $ArCl_2$, a molecular species that is made during collisions of argon atoms and dichlorine molecules in the flowing stream of gas. It can be shown that the lifetime of an individual $ArCl_2$ molecule is about 10^{-12} seconds, time enough for rotation.

On the basis of well-established theory, it is possible to calculate, with a high degree of precision, the *pattern of spectral lines* that should correspond to $ArCl_2$ molecules of various structures. In the experiments recently reported, lines expected for *T-shaped* Ar-Cl_2 show up in predicted positions and *no lines* appear at positions expected for *linear* Ar-Cl-Cl. Not only can we say that a new chemical entity has come into existence, but we can also tell what the shape of that entity is!

Species like $ArCl_2$ are called ‘van der Waals complexes’ because they are held together by relatively weak *dispersion forces* first identified by the Dutch scientist of that name. When two chemical entities (atoms, molecules, etc.) collide, the approach of each *momentarily disturbs the electron-cloud* of the other (*polarization*). Instantaneous distortion of electron-clouds gives rise to opposite electrical charges on momentarily abutting regions of the two collision-partners. Electrostatic attraction of these two opposite charges draws the reactant partners together. This effect is quite weak – a hundredth of usual chemical bond-energies – but it is sufficient to allow the complex to *function as one unit*, at least in so far as rotation is concerned, and therefore the microwave spectrum *of the three-atom aggregate* is observable. *Becoming* of a quite simple sort has occurred in the rapidly flowing gas-stream.

As previously mentioned, it is a common misconception (shared by Connell and van Inwagen) that some entities (perhaps 'particles' of physics) may be regarded as 'simples'. In a previous paper (Earley 1981), I attempted to show that usual interpretations of Whitehead's 'actual occasions' as ultramicroscopic share aspects of this error. High-energy physicists now consider all submicroscopic entities to be one or another kind of *resonance*, with longer or shorter finite duration. These microscopic coherences function as components of larger aggregates, such as the $ArCl_2$ complex. The composition of the smaller units is quite comparable, in many respects, to the coherence of the $ArCl_2$ unit, and $ArCl_2$ could also be part of larger wholes.

Van der Waals molecules (such as $ArCl_2$) in the gas phase are among the simplest chemical species that have the properties that chemists associate with 'existence' (Earley 1992). In these cases, two or three well-understood entities combine in ways that are fully comprehensible, and produce coherences that are capable of unified agency – in this case, absorbing energy from a beam of microwave radiation.

Aristotle considered whether and to what extent a substance can exist *within* another substance. The question of in what sense the components Ar and Cl_2 persist in the compound $ArCl_2$ calls for a complex answer. Methods of inquiry that involve the outer electrons of the constituents indicate that the components have been changed in the complex, but measures that involve only the nuclei and/or inner electrons of the constituent atoms show little or no change caused by chemical reaction.

IV. Transition to Coherence in Nonlinear Chemical Dynamics

It seems likely that the question of what kinds of things are rightly said to be "that which is not predicated of a subject but of which all else is predicated" (Aristotle, *Metaphysics* Z, 1029a 8-9) would generate quite different answers in diverse historical periods, as attention shifts from one sort of coherence to another, and as cultural developments permit new sorts of integrations to come into existence. Brief attention to a second area of current research interest in physical chemistry may be instructive in understanding the becoming of coherences that are important in contemporary culture. Our second example of chemical becoming involves somewhat more complicated systems than our first one did.

Chemical reactions can be carried out in *continuously-stirred tank reactors* (CSTRs), to which reagents are continuously supplied and from which products are continuously removed (by overflow). The state of the contents of such reactors can be monitored by electrical or optical sensors. Under some conditions, the output of the monitoring device varies wildly and in an erratic manner. The pattern of readings in a given time interval *does not repeat*, no matter how long the system is observed. In such cases, it is *not possible* to predict the reading of the sensor at a future time on the basis of information (no matter how precise) on the state of the reactor at a particular time. This condition is called *chemical chaos* (Coffmann *et al.* 1987).

Even for fully chaotic CSTR systems, however, it is sometimes possible to modify one of the conditions of the experiment (to vary pump rate, to change composition of feed-streams, etc.) in a gradual way. In favorable cases, such a change may bring about a progressive simplification of the output signal until, at length, a *fully regular*, simple, oscillation is observed, with a set period of time between succeeding excursions of the recording device. In the chaotic state, oscillations of any frequency are equally probable. (This is expressed by saying that the *power spectrum* of the system has no distinguishable features.) As conditions are slowly changed and recorder-variation becomes more regular, the power spectrum develops characteristic features, and eventually consists of *only a single peak*, indicating that there is *one* frequency that is a characteristic of the set of chemical reactions going on in the tank reactor. As in the $ArCl_2$ case, the interaction of several components has given rise to an observable effect not ascribable to any of the components. This is a kind of *chemical becoming* rather different from that first described.

Many kinds of chemical, physical, and biological organization can come into existence by this route – gradual simplification from disorganized (chaotic) antecedents – and may disperse themselves through the reverse sequence (a *period-doubling cascade*) (Peng *et al.* 1990). Amazingly, there are deep mathematical similarities between sequences of changes that occur in a wide variety of chemical, physical, mathematical, and biological systems. One of the numerical constants involved in many such sequences is almost as well determined as is the value of π.

The predictability and regularity of recurrent behavior in oscillating chemical reactions arise from networks of *feedback loops* of chemical processes. Each of the twenty or more chemical species (molecules, ions, etc.) that is involved in the overall chemical change retains its individual characteristics, and propensities for interaction. The *combination* of all of these characteristics gives rise to the limit cycle – to coherence, and therefore to becoming. In favorable cases it is possible to recognize the set of mathematical relationships *(the attractor)* that is instantiated in the limit cycle. Even in the chaotic case, special techniques can uncover weird kinds of order lurking behind the (real, not only apparent) chaos (Earley 1986).

The harmony indicated by the regular oscillation in state (and single peak in the power spectrum) in such chemical (or other) systems does not result from the kind of reciprocal interaction of components that are in contact (as Aristotle and Leclerc require and $ArCl_2$ exemplifies) but from more-subtle types of mutual influence. The networks of chemical changes that give rise to this kind of organization can be regarded as composed of several parts – several sets of processes, each of which partially controls the others. When these diverse parts of a reaction-network achieve a kind of balance, harmonious oscillation results, and the system *as a whole* serves as a center of agency (the system *as a whole* has a power spectrum) as the $ArCl_2$ molecule does in absorbing microwave radiation. Since, in both cases, the congeries of components functions *as one* with respect to interaction with the external world, to that extent, it *is one*. This is a criterion of integrity that seems as appropriate as any other, and much more satisfactory than the approaches used by Connell or by van Inwagen.

V. Chemical Coherences as Units of Agency

The $ArCl_2$ van der Waals complex makes its presence clear by the *pattern* of lines in the microwave spectrum. That pattern arises from *transitions* of the three-atom aggregate among rotational energy states. The aggregate rotates as a unit because 'dispersion forces' (van der Waals forces) hold the argon atomic fragment and the dichlorine molecular fragment together, however weakly. Those attractive forces are just balanced by repulsive forces engendered when the electron-clouds of the several atomic centers begin to interpenetrate. One can understand the coherence of those individual atomic centers in quantum mechanical terms, but there seems to be no need to get into that level of detail. The net result of all these transactions is that the $ArCl_2$ van der Waals complex is properly considered to exist – to be a real thing, a persisting (albeit briefly) entity, an ontological unit. The $ArCl_2$ van der Waals complex has a dichlorine molecule as one of its components: it is conceivable (but not likely in this case) that such a complex could also be a part of still larger functional wholes. Coherences of the more complex sort described in the later part of this paper can also combine to yield yet larger aggregates (Petrov *et al.* 1993, Hjelmfelt *et al.* 1993).

The coherence in the oscillating chemical system makes its presence felt by the single peak in the power spectrum, corresponding to a single frequency of oscillation. This, in turn, arises from the *closure* of a network of chemical reactions, each one of which has a number of chemical molecular and ionic species as reactants and as products. The fact that some chemical species react while others do not can be understood (in favorable cases) in terms of the chemical bonding (enthalpy) and degree of disorder (entropy) of the reactant and product states. The speed (rates) at which each reaction takes place can also be understood by the application of similar considerations to the intermediate or transition states that intervene between reactants and products. It is the *combination* of the kinetic properties (rate laws and rate constants) of a number of reactions that give rise to the temporal coherence that defines the oscillating chemical system. The oscillating reaction system has a higher degree of complexity than the conceptually simple molecular beam experiment, but in both cases palpable coherence (a new chemical entity) arises from suitable combinations of interactions of prior chemical entities – reactions in the oscillating system and atomic and molecular fragments in the van der Waals complex case. In both these types of chemical system it is possible to investigate the component species or processes in as much detail as may be desired, so that rather complete understanding of those components can be attained. Similarly, the way those components (molecules or reactions) combine to yield coherence is well understood. Even though Connell (1988) regards the formation of sodium chloride as a mystery ("precisely what the character of the interaction is we have no way of determining"), many and various probes are available that reveal to the chemist how the electrons and nuclei move during chemical reactions (the intimate reaction mechanism). The obscurity suggested in the quotation *does not* exist.

Detection of either of the two types of coherence described above requires sophisticated instrumentation – spectrometers capable of recording microwave spectra, or power spectra. But similar considerations apply to any coherence whatsoever. For any interaction between two entities (or more) entities the internal readjustment times (the time constants) of each must be comparable to that of the other. The properties of the 'percipient' (taken in a very broad sense, no consciousness implied, Earley 1995) must be appropriate for the item being perceived, and the characteristic of the item being detected must match (in some sense) the attributes of the item with which it is interacting. This is a universal characteristic of all interactions whatever – not substantially changed by the fact that it is so apparent in these chemical cases.

VI. Dynamic Coherence and Social Structures

Mutually-controlling sets of processes are by no means restricted to chemistry: they abound in economics, sociology, psychology, biology, meteorology, and astronomy. Combinations of these complex types may also be pertinent to understanding high-level structures of wider cultural and philosophic interest. Joseph A. Tainter, an anthropologist who studied the Chacoan civilization of New Mexico, proposed a general theory of the collapse of complex societies (Tainter 1988). In his view, complex societies – characterized by many distinct social roles, number and distinctiveness of parts, effectiveness of control of labor and other resources, and relatively large population size – arise as *problem-solving strategies* that ameliorate conditions of stress. The origin of complex social arrangements often entails economic and hence (usually) reproductive advantage to the human populations that adopt the more-structured ways of living.

Three examples of such organization are the Roman Empire, the Chacoan Culture, and the Maya Civilization. Roman citizens in the late Republic were relieved of taxation by the seizure of the treasury of Macedonia and the steady flow of other resources from the Empire toward the city of Rome. Unusually dry growing seasons in the low regions of the semidesert San Juan Basin of New Mexico generally correspond to wet periods in the surrounding uplands. After the origin of a single (Chacoan) polity encompassing both lowland and upland areas, a surplus in one area could be directed to make up a shortfall in the other region. In the crowded tropical wetland territories of the Maya of Central America, impressive architecture and fearsome art intimidated rival groups.

In each of these diverse cases a specific sort of communal behavior – increasing complexity – had economic (reproductive) advantage. In each of these three cases, enlarging the system that had served the group well seemed to make economic sense; Rome invaded Egypt, the Chacoan economy spread to adjacent areas, several rival Mayan alliances thrived in mutual competition – an art race – after absorbing smaller units (Appenzeller 1994).

But in each case, eventually, diminishing returns applied. Once exploitation of the most accessible resources was completed, the methods (increasing complexity) that had formerly been profitable resulted in losses rather than gains. Strategies that had been highly beneficial in former times (Roman standing armies, Chacoan remote outposts, Mayan ceremonial architecture) imposed costs on the underlying agricultural population that were larger than the benefits gained. This inevitably led to instability, and to the eventual collapse of each system, brought on by one adventitious stress or another. In earlier periods of each civilization, stresses of similar or larger magnitude had been dealt with by each of these cultures by using benefits gained by increase in complexity. In the later stages of the process, increase in complexity gave lower (rather than higher) production. The rational response to stress was for the system to revert to a lower level of complexity – social collapse.

Each of these complex societies is clearly an aggregate made up of many individual humans and numerous artifacts. But each is defined and given identity by a specific *pattern* of behavior that engendered relatively long-lasting coherence – each culture was recognizably continuous over extended periods, even though all the human individuals and most of the artifacts perished and were replaced during those periods. In this sense, each of these coherences is analogous to the oscillating chemical reaction-system discussed previously. If we follow the suggestion of the late Plato, and the practice of experimental chemists, we would count as 'existing' (for some purposes) any patterned set of interrelationships that, under specific historical conditions, yielded coherence sufficiently persistent to have effects (in some specific interaction) as one unified whole rather than as a mere aggregate. With respect to many interactions with the rest of the world, the Roman Empire, the Chacoan trading system, the Mayan Civilization, each functioned as a coherent, fairly long-lived, center of agency. At those times and to that extent, each of these are properly considered units with ontological significance. This radically pluralistic concept is clearly quite different from ontological attitudes inherited from the scientific revolution of the late Renaissance, but is consistent with the practice and direction of contemporary science, and applicable to problems of wider societal interest.

This paper was read at the annual meeting of The Metaphysical Society of America, March 1994, Vanderbilt University, Nashville, TN. The general theme of the meeting was 'Becoming'. Parts of this paper were also read at the Philosophy of Chemistry meeting in Athens Greece in April 1996.

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