The Philosophy of Chemistry Reformulating Itself: Nalni Bhushan and Stuart Rosenfeld's *Of Minds and Molecules: New Philosophical Perspectives on Chemistry**

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Nalni Bhushan and Stuart Rosenfeld (eds.), ***Of Minds and Molecules: New Philosophical Perspectives on Chemistry.*** New York: Oxford University Press (2000), xvi + 299 pp., $60.00 (cloth).

Philosophers of chemistry, following the lead of physicists, have been slow to realize that molecular descriptions issuing from quantum mechanics in the absence of chemical theory are fatally flawed. In the wake of this realization, new topics have begun to unfold—including new metaphysical issues, new concerns about the philosophy of chemistry's place in the philosophy of science, and new accounts of how properties are observed, inferred, and presented. A recent collection of essays, *Of Minds and Molecules: New Philosophical Perspectives on Chemistry* edited by Nalini Bhushan and Stuart Rosenfeld, reveals what some of these new issues are and suggests new directions for the philosophy of chemistry.

1. Subfields are as vital as fields. Within philosophy of science, the subfields of the philosophy of biology and psychology have been thriving for some time, but that of chemistry is just beginning. One of the reasons for this late start has been the expectation—fostered by physicists such as Dirac—that molecular descriptions could be derived from just the laws of physics

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(Dirac 1929). However, the fundamental theoretical basis of chemistry, quantum chemistry, continues to rely heavily on chemical theory, without which quantum chemistry cannot even approximate the shapes of molecules. Bereft of what many thought should be its central aim, showing how chemistry is a part of physics, the philosophy of chemistry is "reformulating" itself.

As is made clear in the introduction to the volume as well as in many of the articles, the Dirac/quantum mechanical tradition, continuous with philosophy of physics, is just one of two prior traditions. The other is antireductionist and conceives of chemistry as an autonomous discipline. The reformulation that this volume suggests is an attempt to find a "third way" between these extremes.

2. Metaphysics of Chemical Substances. This topic, one of the three main developing subjects in the philosophy of chemistry, concerns the identity and persistence conditions of atoms and molecules. On almost any chemist's account, a molecule retains its identity when it changes shape through vibrations and rotations but loses its identity when covalent bonds are broken or formed.

That shape—or a range of shapes limited by vibrations and rotations—is necessary to the concept of molecular identity would seem to go almost without saying. Yet some of the accounts of molecular identity suggest otherwise. Jeffry Ramsey, for example, argues that shape is not an aspect "essential" to molecular identity. This is a consequence of the fact that, since molecular observation often takes longer than the vibrations or rotations of the molecules being observed, molecular shape sometimes appears blurred. Consider, for example, a methyl group which, freely rotating at room temperature, can be slowed down by lowering its temperature through the use of a low temperature beam. When the molecule is observed using an X-ray crystallographic instrument in combination with a low temperature beam, the rotation of the methyl group is slowed and the position of each hydrogen may be relatively well defined. In the absence of the beam, the methyl, freely rotating, may appear as just a sphere (see Vollmer 2003).

On Ramsey's account, the shape of the methyl is the shape its atoms sweep out during an observation. This means that the methyl, in his view, has a different shape when observed at room temperature than it does when observed with a low temperature beam. Since molecular shape depends on conditions in this way, then, shape "does not 'belong' essentially to matter as a 'basic' physical feature." Ramsey concludes that the idea that "molecular shape is essential" is false (Ramsey 2000, 122).

There is, however, a problem with Ramsey's argument. On his account, the shape of a baseball that is thrown through the air is either a long

streak or a small sphere, depending on how we observe it. But the shape of a baseball, at least as we ordinarily use the word, is a small sphere and not, depending on conditions, sometimes a long streak. Therefore, Ramsey's use is confusing. If there is reason to adopt a different account of shape—when it comes to molecules—than the one we use in ordinary observation, then we need an explanation of why, as well as an explanation of just how the new account of shape differs from the old one (see Vollmer 2003).

Ramsey also argues against the significance of shape in molecular identity on the basis of a certain method of providing a quantum mechanical description of molecules (Woolley 1985). On this approach, one does not feed in any information from chemistry about the structure of molecules, such as the relative positions of nuclei (bond lengths and angles). As a consequence, the resulting descriptions designate no shapes at all—nor any parameters that are placeholders for shape. To understand the significance of this, one should remember that any collection of isomeric molecules, such as n-pentanol, 2-pentanol and isopentanol, all have the same number of atoms of each kind (in this case five carbon, one oxygen, and twelve hydrogen) and the same numbers of electrons. The isomers differ from each other, then, only in the relative positions of the nuclei and electrons. Since they differ in this way only and since on this kind of quantum mechanical approach no shapes, nor placeholders for shape, are derived, they differ not at all. This means that a single quantum mechanical description, surprisingly, designates all three species. Some speculate that such a description is complete and therefore that molecules as they are described by quantum mechanics—complete isolation from other molecules and from photons—really have no shape.

Because molecules are never isolated under the actual conditions of an experiment, it might at first seem that having no shape in isolation can be consistent with a chemical theory that typically deals with aggregates of molecules. Yet there are serious inadequacies with this approach. Suppose a drop pure in one isomer, say, n-pentanol were converted to a gaseous form so rarified that the molecules were in isolation. Then the quantum description would become appropriate, a description which has no shape and no placeholder for shape. It must describe, then, not just n-pentanol, but 2-pentanol and isopentanol as well. Furthermore, if the description is complete, this suggests that the isomers of pentanol are identical in every way. If the gas were to contract and the molecules were to come out of isolation, the standard chemical description would again become appropriate. However, since in chemistry there are three different pentanols, how would we know which one(s) to expect in the drop that had been n-pentanol before isolation? If the answer is that we could expect n-pentanol to reappear in the drop, then information about shape would have to have

been carried through into the quantum mechanical description—how else could the drop of n-pentanol reappear? If, on the other hand, we could not know which isomer to expect, then this is inconsistent with chemical theory—isolation alone does not cause isomers to interconvert.

Ramsey's response to these quantum mechanical descriptions is to accept their completeness. Under some conditions, he says, a molecule has "no nuclear frame" (2000, 119). Molecular shape is, therefore, "not primary, not essential, and not real" (125). His view that molecular shape is "not real" is actually more complex than one might think from this quotation. He expresses a second, contrasting, view, that molecular shape is real in "most circumstances," or that it is more often real than not real (123). It is unclear which of these two claims, on balance, better represents his view. Either way—whether molecular shape is not real or only sometimes not real—this poses a difficulty, Ramsey suggests, for the classical concept of molecular shape and since science cannot do without it, "metaphysics should give way" to science (123).

In a similar vein, Andrea Woody and Clark Glymour in this volume express the view that "the classical notion of molecular shape" that many assumed to be consistent with quantum mechanics "has been placed in doubt" (2000, 19). If this means that what is in doubt is the classical descriptions, then we ought to ask why we should assume the quantum mechanical descriptions are complete and therefore doubt the classical ones, the only ones that can account for such things as differences in the properties of isomers, their products along various reaction pathways, and the diffraction patterns of their crystals. Alternatively, if Woody and Glymour mean that we ought to doubt the classical notion of shape, not just as it applies to molecules, but as it applies to objects of all sizes, then this doubt is part of the larger question of what we mean when we describe a quantum world in classical terms, and not a question specific to the issue of molecular identity.

The question of the importance of shape is part of the larger metaphysical issue of what we mean by molecular and elemental identity. This more general question is taken up in a paper by Eric Scerri which analyzes Fritz Paneth's account of the concept of element (Paneth 1962). Paneth notes that the creation of a new substance by mixing two known substances is prima facie incomprehensible. However, what looks like coming into being and ceasing to be, as the atomists first realized, can be reduced to a logic that retains an underlying, unchanging substratum—permanent atoms. The account Paneth offers requires, surprisingly, the existence of a strange kind of entity: the qualityless atom.

On Paneth's account, an elemental substance has apparent properties such as its color. However, when an element, x, reacts in an ordinary chemical reaction with y to form the compound x-y, the apparent properties of x and y disappear to be replaced by the apparent properties of x-

y. Since x by definition remains unchanged, its properties ought to remain unchanged. Therefore, the apparent properties of x are not its real properties. Paneth suggests that all the properties of x are of this kind—they disappear on chemical transformation. What Paneth means by properties in this context are all the properties of interest to chemists, including taste, odor, feel, color, and valence (1965, 8). These are the properties, he says, that are generated only by "the coming together of many atoms" and that are, therefore, not discernible in the individual atom, such as an individual atom of gold (13).

There are, however, other properties, hardly mentioned in the paper, that exist independently of the atoms coming together. Paneth explains in a footnote that these properties include those of the nuclei, such as atomic weight. In the wake of Rutherford and Bohr, Paneth suggests, it was realized that this kind of property signals "the unchanged presence of all atomic *nuclei*" which explains the "persistence of an element in its compounds" (1962, 152 n. 3; his emphasis). A puzzle, then, arises. The persisting properties, which explain the persistence of an element and therefore the identity of a chemical element are, Paneth's implication seems to be, properties that are not of interest to chemists!

Scerri does not resolve this puzzle. Indeed, he compounds it. Scerri reports that when isotopes were discovered, elemental identity was switched—partly through Paneth's influence—from identification with atomic weight to identification with atomic number. Scerri says of the switch that, if atomic weight was problematic, as it was after the discovery of isotopes, "it was because it [atomic weight] was not a chemical property" (Scerri 2000, 70 n. 44). This suggests that the switch was made from atomic weight to atomic number because atomic number was a "chemical property" whereas atomic weight was not. However, since both are persisting properties of the nuclei, neither would seem to be, on Paneth's account, a property of interest to chemists. Therefore, it is hard to know what Scerri means by suggesting atomic number is a chemical property and, thus, hard to know whether Scerri agrees with Paneth about which properties are of interest to chemists. It is also hard to know which properties Scerri takes to be the physical, as opposed to the chemical ones or whether he thinks the difference is important.

Whatever view one takes with respect to Paneth's definition of the chemical properties, he is right in claiming that the terms for the elements are sometimes used to refer to atoms individually and other times to refer to atoms jointly as a substance. "Sodium," for example, can refer to either individual Na atoms as they exist in metallic Na (or NaCl) or to the elemental substance Na with its metallic properties. In the former case "sodium" refers to such properties as atomic number and weight; in the latter case, it refers to the ordinary secondary properties of elemental sodium.

One possible way to clarify our terminology would be to think of the

nuclei and inner electrons, or "kernel," of sodium as the real sodium itself—this is the part of sodium that is both unique to Na and persists, more or less, through chemical change. Alternatively, "Na" could refer to the entire Na atom, including its outer electrons. While the choice of the entire atom as referent may seem a more natural one, on this meaning, "Na" would refer to a chemical form that is both various and changing—since Na^0 can convert to Na^{+1} and vice versa. If "sodium," on the other hand, were to refer to only the kernel, it would thus refer to an underlying substrate that is more or less unchanging. Of course, however we decide the issue, the answer to the question, "How much sodium is present in this substance?" will remain the same. In any case, this distinction is of fundamental importance and, if our use of the terms for elements were to better reflect it, our basic chemical concepts would become more clear.

3. Autonomy of Chemistry. This is the second of the three main developing topics in the philosophy of chemistry. The central issues include reductionism, the theory independence of data, and realism. In this volume, Eric Scerri, for example, raises the question of whether atomic orbitals "really exist" in accordance with their scientific descriptions or whether they are just heuristic devices accounting for observable phenomena, such as spectroscopic observations. Scerri sides with those who favor the latter interpretation—atomic orbitals do not really exist. However, Scerri's sympathies do not lie entirely in this direction because whether an orbital term refers is determined, in his view, by whether it can be derived from quantum mechanics. That this is Scerri's view is suggested by his claim that to say orbitals do not really exist is to say that the terms for them "cannot be reduced to quantum mechanics" (2000, 52). By reduction to quantum mechanics, he means derivation from a quantum mechanics, all the terms of which are from physics. He suggests, then, that on this basis, the single-electron orbital terms, such as that for the hydrogen atom, refer, whereas the multi-electron orbital terms, nearly all the rest, do not.

Scerri's claim—whether an orbital term refers is determined by whether it can be derived from quantum mechanics—may be a narrow claim just about orbital terms. Such a claim is likely to be justified by the broader claim that a scientific term—of any kind—that refers must be derived from quantum mechanics. If Scerri's narrow claim is, indeed, justified by this broader one, then we need to know why we should accept the broader claim, that is, privilege the terms of quantum mechanics over other terms.

One reason to privilege terms which can be derived from quantum mechanics might be that they are, as Scerri suggests, uniquely well defined. However, as he realizes, being well defined is not a standard condition for reference. For example, a stellar phenomenon, if it existed long ago and far away, may be only approximated, yet reference would not be denied

on this basis. His discussion of the reference of orbitals, thus, may simply reflect a strong commitment to physics.

Others in this volume, including Maureen and John Christie, defend a pluralistic chemistry that suggests that the terms of quantum mechanics must be supplemented by chemical theories of various kinds. The Christies and Barry Carpenter also suggest that, in science, parallel, competing descriptions can be accepted simultaneously within a single tradition, each one in a partial or conditional way. Jaap van Brakel explains in this volume that not only are quantum mechanical terms—whether supplemented by chemical theory or not—not privileged over chemical ones, neither kind is privileged over our ordinary terms for the macroscopic world.

A final topic showing the relevance of chemistry for general philosophy of science is the question of whether observation is possible that is independent of theory. In his essay, William Lycan suggests that the chemical senses—taste and smell—involve inductive reasoning, but ordinary sight does not. When we see objects, he explains, we seem to be presented, simpliciter, with the objects themselves; however, in tasting or smelling, we do not seem to be presented with them. This might raise the question of whether analyzing sight into an initial uninterpreted experience followed by a subsequent interpretation could provide the basis for an account of perception on which the various senses would be more on a par epistemologically.

4. The Observation and Presentation of Chemical Properties. Various papers in this volume are concerned with how chemical properties are observed, how inferences are made, and how substances are represented. Steve Weininger, for example, suggests in this volume that when we think of the representation of a substance, we typically think of a presentation of its structural attributes, such as the atoms of which it is composed and their arrangement in space. However, bulk properties can represent a substance as well, as in the case of a phase diagram or a picture showing the substance's macroscopic appearance—such as the white cubic crystals of NaCl. The two kinds of properties, however—individual properties and bulk ones—are rarely apparent in the same context. Emily Grosholtz and Roald Hoffmann note that, when a substance is referred to in a scientific paper by a term, such as "benzene," the term does not always signify the structure, but sometimes a substance's bulk properties, such as being a clear liquid, having a boiling point of 80°C, and having a vapor pressure of 0.1252 atm. This, Grosholtz and Hoffmann say, creates an ambiguity.

That terms sometimes refer to bulk properties regardless of microstructure may, many think, be true of common names. However, in Putnam's view, as argued in this volume by Stuart Rosenfeld and Nalini Bhushan, this is not true even of common names. This is because, in Putnam's view,

the microstructural properties of a substance are factored into the meaning of the terms that pick it out at the macro level (2000a, 200). Although Putnam may be wrong with respect to common names, about most chemical terms he is not. A chemical term rarely, if ever, refers only to bulk properties without any implication regarding underlying structural attributes. Therefore, by the ambiguity of a term such as "benzene," Grosholtz and Hoffmann would seem to mean lack of certainty about which properties—bulk or structural—are relevant in a given instance. Knowing which ones are relevant, they suggest further, is something chemists take for granted.

Many of the properties known by chemists have been learned through the use of instrumentation, the goal of which, as described by Davis Baird, is not always greater precision but, as suggested by Daniel Rothbart, is usually the correlation of macroproperties, such as wavelengths of absorption peaks, with microstructural characteristics. What chemists know about micro properties, Woody and Glymour argue, results from chemical inference based on the observation of macroproperties. An example given is the calculation of atomic weights from vapor densities by Cannizzaro.

Because many of the papers in this anthology are co-authored by philosophers and chemists, these papers are, by and large, both philosophically and scientifically informative. Collectively, the authors have produced a volume that helps to illuminate the metaphysics of the philosophy of chemistry, the place of chemistry in philosophy of science, and the ways chemists observe and infer. A birth is in progress: philosophy of chemistry is arriving to take its place in the world of ideas. The authors of this volume are helping to make it happen.

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