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Microstructure without Essentialism: A New Perspective on Chemical Classification

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Recently, macroscopic accounts of chemical kind individuation have been proposed as alternatives to the microstructural essentialist account advocated by Kripke, Putnam, and others. These accounts argue that individuation of chemical kinds is based on macroscopic criteria such as reactivity or thermodynamics, and they challenge the essentialism that grounds the Kripke-Putnam view. Using a variety of chemical examples, I argue that microstructure grounds these macroscopic accounts, but that this grounding need not imply essentialism. Instead, kinds are individuated on the basis of similarity of reactivity between substances, and microstructure explains similarity of reactivity.

1. Introduction. The microstructural account of the individuation of chemical kinds was taken as the received view in the literature on chemical kinds in the decades following Putnam's (1975) and Kripke's (1981) proposals that gold is the substance with the atomic number 79 and that water is the substance made up of H_2O. While Kripke's and Putnam's views differ in important ways, they agree that (1) the essences of chemical kinds are microstructural and that (2) individuation is a matter of sorting kinds according to their essences. So for Kripke and Putnam, microstructural essentialism, the view associated with statement 1, grounds the individuation of chemical kinds.

A recent movement in philosophy of chemistry has challenged microstructural essentialism, arguing that microstructure is unnecessary for the individu-

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ation of chemical kinds and so is inessential to chemical identity. Instead, proponents of the alternative view argue that (1) patterns of reactivity provide the appropriate criterion of individuation and that (2) microstructure is too diverse and complex to effectively capture patterns of reactivity among chemical kinds. This view has been championed especially by Van Brakel (2000), Needham (2000, 2011), LaPorte (2004), and VandeWall (2007). Each of these authors has used reactivity-based individuation to reject microstructural essentialism, and each develops a nonmicrostructural account of individuation. Needham, for instance, argues that complex chemical substances such as water should be individuated thermodynamically, which amounts to individuation by macroscopic properties such as "the different volumes of equal masses in the gas phase at the same temperature and pressure" (Needham 2011, 11–12). Taking a more operational line to arrive at the same conclusion, Van Brakel argues that "the chemical notion of substance is wholly defined in terms of laboratory procedures and other experimental practices, and can be given no essentialist definition. Any identification of a particular substance may change under the influence of new observations, including observations using spectroscopic techniques and similar (sub)microscopic methods. But the final arbiter will, in the end, be observations at the macroscopic level" (Van Brakel 2000, 73). These reactivity accounts of chemical kind individuation thus urge a "macroscopically oriented account of sameness of kind" (Needham 2000, 21) in response to the failure of microstructural essentialism.

While these accounts provide convincing arguments against microstructural essentialism, they are too hasty in moving from the failure of microstructural essentialism to the rejection of microstructure as a tool for individuating chemical kinds. Microstructure is one of the hardest-working explanantia in chemical theory, and it can be used to justify observations about patterns of reactivity, as well as to make predictions about reactive behavior and to explain whether and when two apparently similar reactions are in fact of the same kind.

This essay proposes a new account of chemical kind individuation that reconciles the microstructural account with the reactivity account. While the reactivity account correctly identifies the need to individuate chemical kinds according to patterns of reactivity rather than microstructural essences, it is too hasty in dismissing microstructure in favor of macroscopic descriptions of reactivity. I show that it is both possible and fruitful to recover the microstructural account without clinging to microstructural essentialism. My account uses reactivity rather than microstructure as the fundamental individuation criterion for sameness or difference of kind, but it shows that differences in reactivity are due to differences in microstructure, once microstructure is understood to include molecular geometry. This new account of microstructure can not only individuate kinds by reactivity, but it can also

identify useful relations among kinds that cannot be predicted on the basis of macroscopic properties alone. Further, establishing reactivity in terms of microstructure accords with the chemical practice of modeling reactions in terms of molecular composition and changes in molecular structure, thus preserving the individuation practices of the science itself.

This account differs in philosophical intent from the discussions of microstructural essentialism found in Kripke and Putnam. Those authors employed microstructure to ground discussions of essences, which were in turn used (and used differently by each author) as jumping-off points for their theories of semantic content. Consequently, the fact that their discussions turned to chemical kinds was largely incidental to the greater philosophical projects. The account presented here, on the other hand, is about chemical kinds in their own right. Its implications for the broader conversation about semantic theory are incidental, although perhaps not inconsequential. Whereas the mechanics of essences mattered much for Kripke and Putnam, essences are important to this account only to the extent that they affect chemists' ability to classify. One of the aims of reconciling the microstructural and reactivity accounts, then, is to show that discussions of essences can be construed as largely orthogonal to questions of chemical classification; in other words, microstructure is used here to ground a pragmatic—rather than a metaphysical—account of chemical classification. Such an account can easily supervene on a realist, essence-based theory of chemical kinds, but it need not appeal to such a theory to get off the ground.

The argument proceeds as follows. In section 2, I defend the motivation of the reactivity account and define sameness and difference of reaction. Section 3 identifies two kinds of chemical microstructure already in the literature and introduces an expanded notion of chemical microstructural properties, which includes the notion of a molecular-geometric property. Section 4 argues that changes in microstructure ground changes in reactivity. Section 5 applies this hybrid account of chemical kind individuation to examples that have in the past served as critiques of the microstructural account or of microstructural essentialism. I show how these examples can be accommodated by a more nuanced notion of chemical microstructure and, in particular, how my account offers a novel take on the perennial problem case of water.

2. Reactivity Determines Kind Membership. In this section, I follow the reactivity account in arguing that reactivity is the appropriate basis of individuation for chemical kinds. I discuss how to characterize a chemical reaction and how to determine sameness of kind via sameness of reaction. Then I demonstrate that any finer- or coarser-grained principle than sameness of reaction is either insufficient or unnecessary. Recognizing this motivates the following two sections, in which I discuss how an appropriately thick notion of chemical microstructure can be used to justify observations

and predictions of sameness of reaction and, thus, sameness of chemical kind.

An intuitive principle of individuation for chemical kinds aligns the same-kind relation with a test of sameness of function in chemical reactions. In other words, some sample K bears the *same kind as* relation to another sample L just in case K enters into all the same chemical reactions as L enters into, and no others. All the same chemical reactions (hereafter ASCR) is a purposely vague relation, and some elaboration will make it clearer what falls under its umbrella and what fails to: ASCR includes the test of whether or not every substance that can be combined with K can be combined with L and whether or not the products of such combinations are the same in the two sets of cases. The tests here are assumed to take place under identical background conditions. This principle of individuation is both intuitive and discipline-specific, ensuring that the identities and differences it produces are chemical identities and differences rather than, for example, physical or biological identities or spurious differences.[1]

It is difficult to see how a coarser-grained principle would suffice for the individuation of fundamental chemical kinds, because by definition a coarser-grained principle would permit the *same kind as* relation to hold between two samples that enter into different chemical reactions. No matter what additional restrictions were put on such a principle, it would still permit kind-identities between things that play different roles in chemical processes. So a kind picked out by such a principle could have a disjunctive and even an internally contradictory set of chemical properties—for instance, such a kind might have both the property of being water soluble and that of being water insoluble, depending on the sample. Such a kind is useless for the practice of chemistry, because it does not help a chemist to determine which bottle to grab off the shelf in the laboratory.

So no useful principle of chemical kind individuation can be coarser grained than ASCR. What of a finer-grained distinction, such as one where two samples must have similar size or shape in order to be of the same kind? Sometimes, the size and shape of a sample affects whether or not two samples participate in all the same chemical reactions. For instance, a sample of ${}^{235}_{92}\mathrm{U}$ of higher-than-critical radius will be physically unstable, which will interfere with its ability to chemically react with another substance. Similarly, small

1. Many chemically identical substances may also exhibit physical identity, biological identity, both, or neither. The discipline-specificity of ASCR is meant not to rule out relations between chemical identity and identities conferred by other disciplinary needs, but rather to permit nonchemical differences between substances (e.g., the sample's mass, the angular momenta of nonbonding electrons, or differences in base-pair sequencing in proteins) that would make two samples physically or biologically distinguishable but reactively indistinguishable. I thank an anonymous reviewer for bringing my attention to this point.

samples of many materials, such as nanoscale materials, are physically unstable relative to larger samples of the same material. This instability arises as a consequence of changes in surface structure and the proportion of the atoms in a material that lie on the material's surface (Hornyak et al. 2008, 295–96). This instability generally increases the reactivity of nanoscale surfaces relative to bulk-scale surfaces, which means that many nanomaterials have to be stabilized by being coated in another chemical substance. This coating is necessary to prevent the materials from growing above the nanoscale, and it can interfere with the material's reactivity.[2]

When sample size affects the ability of substances to participate in chemical reactions, then size is a factor in determining whether two samples of a material participate in all the same reactions. In each of the above cases, changes in the size of a sample lead to changes in the reactivity of the sample. Importantly, these changes in reactivity are usually explained in terms of changes in the sample's microstructure: a nanoscale sample of gold has a less stable surface microstructure than macroscopic gold, which accounts for the different reactive properties described above. Likewise, once the $^{235}_{92}U$ sphere achieves critical radius, atoms that make up the sample radioactively decay in a chain fission reaction. This in turn changes the reactions in which the material can participate by changing the (microstructural) elemental identity of some of the atoms in the sample. In cases of this sort, it often makes sense to treat samples of different sizes as different kinds, and this is, in fact, what chemists do: nanoscale gold spheres are termed "colloidal gold" or "gold nanoparticles," rather than simply "gold," and $^{235}_{92}U$ that has decayed is identified as a mixture of its various decay products, including $^{141}_{56}Ba$ and $^{92}_{36}Kr$. These explanations of changes in reactivity due to surface structure and radioactive decay could not be obtained on the basis of observations of macroscopic chemical behaviors alone, and so the role of microstructure in explaining and justifying changes in reactivity begins to become apparent.

Sometimes the size or shape of a sample does not influence ASCR but does still affect some aspect of a chemical reaction, namely, the reaction rate. For instance, the difference in size between a tablespoon of baking soda ($NaHCO_3$) and a cup of baking soda does not affect the reactions in which the soda can participate; both a tablespoon and a cup of baking soda will react with vinegar to form the classic science-fair volcano. But this kind of difference does affect how a chemical reaction occurs. Changing the relative quantities or concentrations of reactants will influence how quickly a reaction proceeds and whether it proceeds to completion. For example, it takes significantly less time for a teaspoon of baking soda to dissolve in a gallon of vinegar than it does for

2. Interestingly, nanoscale gold spheres are an excellent example of materials that need external stabilization, which raises quite an eyebrow against philosophers' historical use of the size of a gold sphere as an archetypical contingent property.

a tablespoon of baking soda to dissolve in a cup of vinegar. However, in both cases dissolution is explained in terms of the same microstructural movements in the component molecules: the ionic bond between sodium and chlorine breaks as a consequence of exposure to polar water molecules, and no new chemical species appear as a consequence of slowing down or speeding up the rate of reaction.

There is a further reason to accept the microstructural justification of ASCR. In addition to individuating fundamental chemical kinds, ASCR provides a foundation for individuating higher-level chemical kinds. For instance, kind terms such as "halogen" and "alkali" pick out not single substances but families of substances. Substantially distinct members of these families do not meet ASCR, but they do overlap in many of their reactive behaviors and so may be said to participate in many relevantly similar chemical reactions. For instance, lithium (Li) and cesium (Cs) are both alkali metals. They both form salts with electronegative elements such as fluorine and chlorine, they both readily oxidize (corrode) upon exposure to air, and they both react violently upon exposure to water.[3] However, where cesium readily reacts with graphite, a form of carbon, to form electrically conductive compounds known as graphite intercalation compounds, lithium does not in general form intercalation compounds, and when it does, the ratio of lithium to carbon differs from the ratio of cesium to carbon (LiC_6 vs. CsC_8; Ohzuku, Iwakoshi, and Sawai 1993). As I discuss at more length in section 3.2, similarities in reactivity are explained by the possession of shared microstructural properties—for instance, in the case of alkali metals, the possession of a single electron in the elements' outer valence shells.

Finally, it should be noted that some transformations of substances that are indispensable to chemistry, such as the melting of a metal, are nonetheless not chemical reactions. What makes a reaction chemical is a question best answered by the standards of chemical practice: chemists' "Gold Book," a compendium of standard definitions of chemical concepts put out by the International Union of Pure and Applied Chemistry, considers a reaction to be chemical just in case it is "a process that results in the interconversion of chemical species" (Muller 1994, 1077). Similarly, a leading introductory chemistry textbook defines a chemical reaction as "processes in which one or more substances are converted into other substances" (Brown et al. 2008, G-3). Given that the aim of discussing chemical reactions here is to use them to individuate chemical species or substances from one another, this definition

3. Upon contact with water, all alkali metals rapidly form hydroxide compounds, releasing hydrogen gas and generating heat. Often this combination will lead to ignition of the hydrogen gas and, consequently, an explosion. These effects are more pronounced for heavier metals than lighter ones, so where lithium's reaction can spark a small flame, cesium's reaction looks like fireworks and is so explosive that it necessitates shielding of the reaction site.

threatens circularity—but not viciously so. While the motivation for chemical kind individuation comes from the desire to individuate the kinds that enter into different chemical reactions for the sake of accurately reflecting the practice of chemistry, what justifies this individuation is still microstructure. How this justification works is the subject of the next two sections.

3. Refining Chemical Microstructure. I have argued that fundamental chemical kinds should be individuated such that no two kinds enter into all the same chemical reactions and no two members of one kind enter into different reactions. But standard definitions of chemical reactions involve reference to changes in chemical substance, so to avoid vicious circularity, an alternate criterion than just ASCR must be used to rationalize chemical similarity and difference. In this section, I argue that chemical microstructural properties provide such a mechanism by explaining differences in reactivity. To make this argument, I discuss what sorts of properties should be counted as chemical microstructural properties (CMPs), in particular defending a somewhat broader definition of CMP than traditional examples of CMPs such as atomic number and compositional formula. I argue that molecular-geometric properties should be counted among CMPs because they capture microstructural variation on par with differences in atomic number.

It has been pointed out before (see, e.g., Needham 2000, 13) that there is no one standard definition of chemical microstructural property, although microstructural properties are frequently characterized by contrast with macroscopic, observable properties. When more detail than this contrast is given, CMPs are generally spelled out by way of examples. The examples of gold and water have become particularly prominent in the philosophical literature, and these examples each illustrate different types of CMPs. I use these examples as a foundation for a definition of chemical microstructure; then I add the notion of molecular geometry.

3.1. Two Types of CMPs. Defining "gold" as "the thing with the atomic number 79" illustrates the first type of chemical microstructural properties, which I will call *monadic CMPs*. Monadic CMPs deal with the structure of individual atoms. While atomic number, or the number of protons in an atomic nucleus, is the most frequently discussed of monadic CMPs, other properties internal to individual atoms also make a difference to chemical microstructure. The number of neutrons in an atomic nucleus determines which isotope of an element is in a sample, and differences in isotope affect chemical reactivity. This point can be illustrated by the example of uranium, whose two isotopes, ${}^{235}_{92}\mathrm{U}$ and ${}^{238}_{92}\mathrm{U}$, differ in reactivity such that the former is fissile and the latter is not.

Another aspect of chemical reactivity that is determined by monadic CMPs is the number of electrons in an atom. If an atom has an unequal number of

electrons as compared with protons, it is an ion and as such is more likely to enter into certain electrostatic bonds with another atom. Thus, it enters into different chemical reactions than its neutral counterpart, so it should be considered a distinct chemical kind.

The second kind of chemical microstructural property already in the literature is exemplified by the case of water being defined as the thing with the chemical formula H_2O. CMPs of this sort deal with relations between atoms, so I will call them *relational CMPs*. The most commonly-referenced relational CMPs are ratios of species of atoms in a compound, such as 2 hydrogen:1 oxygen.

However, an example will illustrate why compositional ratios are insufficient to individuate fundamental chemical kinds. The drug thalidomide was prescribed as a sedative until it was found responsible for a number of radical birth defects (Lenz 1988). It was later discovered that thalidomide, $C_{13}H_{10}N_2O_4$, has two stereoisomers—that is, two different geometric arrangements that are not superimposable. These two isomers (also called enantiomers) are mirror-image versions of one another, like the left hand is a mirror image of the right. The difference between the two isomers is not one that can be accounted for by counting the components of the molecules nor the components of any part of the molecule; it arises instead from the nonsuperimposability of structural relationships in the two isomers. But that difference makes a difference: one isomer of thalidomide was shown to be responsible for the birth defects and the other for the sedative effect the drug was intended to produce (Ratcliff and Eccles 2001, 170).

While the effects are more pronounced at the biological level than the chemical level, it is clear that the two stereoisomers engaged in different reactions to produce such divergent effects. Thus they are distinct chemical kinds, but because they have identical chemical composition they meet the criteria for the same chemical kind as given by this first-pass formulation of relational CMPs. Their distinctness can be recovered, however, by expanding the formulation of what it means to be a relational CMP to include molecular-geometric properties. This is the expansion of chemical microstructure that is needed to individuate chemical kinds such that each fundamental kind meets the ASCR principle.

Relational CMPs are perhaps of most use in organic chemistry, where chemical formulae can underdetermine molecular structures. Many chemical formulae, including that of H_2O, embed information about molecular geometry—"H_2O," for instance, immediately calls to mind the bent, "Mickey Mouse" geometry of a water molecule. However, the existence of classes of structurally underdetermined chemical formulae, such as the stereoisomers described above and the allotropes of phosphorus described below, grounds the need for relational CMPs.[4]

4. I thank an anonymous reviewer for bringing this point to my attention.

3.2. Molecular-Geometric Properties. Molecular-geometric properties are properties that express particular kinds of spatial relations between electronically interacting atoms in a molecule.[5] These properties are attributable to the bonding behaviors of molecules, which produce regular and reproducible three-dimensional arrangements. For example, it is well known that methane (CH_4) is tetrahedral: hydrogen atoms surround a central carbon, orienting themselves at the four corners of a tetrahedron, each about 109° apart.

Properties like methane's tetrahedral shape, as well as the distance between the central carbon and each of the hydrogen atoms, are molecular-geometric properties. They express spatial relations between atoms in a molecule or crystal, treating molecules as more complex than mere clumps of atoms. This kind of description is available to any molecule: as soon as one atom bonds with another, it is possible to describe the bond as more than just the juxtaposition of two atoms. One does so by describing features such as bond energy, bond length, and bond angle.

These properties are microstructural, because they describe features of the material that are only apparent at length and time scales well below the limits of macroscopic (i.e., naked eye) detection. They are similar to the relational CMP used by Putnam to individuate water, insofar as they deal with relations between atoms. But whereas describing water as H_2O gives nothing more than a compositional formula—that is, a simple ratio of clumps of atoms, with no comment on the spatial arrangement of those atoms—adding molecular-geometric properties to relational CMPs permits further elaboration on the geometry of a chemical substance.

This further elaboration rationalizes the individuation of chemical substances by ASCR, explaining why all members of a kind engage in all and only the same reactions. Without the addition of molecular-geometric properties to the class of things that count as chemical microstructure, substances with radically different reactive behavior could not be distinguished from one another. As an example, consider the element phosphorus. Phosphorus has a number of allotropes, which are different arrangements of bond lengths and bond angles that are correlated with different physical and chemical observable properties. The allotropes of solid phosphorus include white phosphorus and violet phosphorus. White phosphorus is composed of tetrahedral arrangements of four atoms, and among its interesting chemical properties is its ability to spontaneously combust in air during warm weather, beginning at temperatures of about 30°C. It also dissolves in some common

5. I include under this heading crystal lattice structures, which are only loosely characterized as "molecular," but which nonetheless are relational chemical microstructural properties that define spatial relationships among electronically interacting atoms.

solvents, such as benzene and sulfur monochloride. Violet phosphorus is crystalline. It does not combust at temperatures below 500°C and it is not soluble in any common solvent.

These reactive differences suggest that the two allotropes should be considered distinct chemical kinds, because they are discernible according to the ASCR criterion. But the individual atoms of each kind of phosphorus can have all the same monadic CMPs.[6] Further, the substances can be composed of clumps of atoms of the same size, so CMPs of the initial relational type, which pick out merely compositional ratios with no consideration for internal molecular geometry, would classify the two kinds of phosphorus as identical.

But with the additional characterization provided by molecular-geometric properties, the difference is easy to see. White phosphorus is tetrahedral, which here means molecules of white phosphorus are composed of groups of four atoms that are distributed spatially as if at the four corners of a trigonal pyramid. Violet phosphorus, on the other hand, is crystalline, meaning it takes on a geometry in which all atoms of a crystal are bonded into one macroscopic molecule. The geometry of violet phosphorus's crystals is such that atoms are located at the corners of rectangular prisms. The molecular-geometric properties of white phosphorus and violet phosphorus differ, and this difference explains differences in reactivity while providing a microstructural basis for discernibility of one substance from the other. No other microstructural properties need differ, so without molecular-geometric properties, the substances could not be individuated microstructurally.

Not only is it possible to individuate molecular species in these terms, it is what chemists in fact do on a regular basis. Tables of internuclear distances and descriptions of common molecular geometries are present in any basic chemistry textbook. Experiments to determine bond angles and distinguish molecules of identical composition based on their internal geometries take place regularly. Adding molecular-geometric properties to the class of relational CMPs both reflects chemical practice and permits further individuation of chemical kinds into partitions that conform to the ASCR principle, whereas leaving molecular geometry out of the picture does not. Only by including molecular-geometric properties as a part of chemical microstructure can a microstructural individuation of chemical kinds correlate with the ASCR principle.

So far, I have been primarily concerned with individuating fundamental chemical kinds by the ASCR principle using this new notion of chemical microstructure. While this will remain the focus of the present discussion, it

6. All the atoms of a sample of phosphorus need not have all the same monadic CMPs, though, as there are multiple isotopes of phosphorus.

should be mentioned that individuation by reactivity, justified in microstructural terms, can and does occur at higher levels in chemical taxonomy. One need look no further than the periodic table of the elements to see such individuation. Take, for instance, the first vertical column of the standard table, which is known as the group of alkali metals. The term "alkali metal" picks out a monadic microstructural property, namely, the presence of exactly one outer-shell electron in atoms composing neutral samples of the element, which is common to each element that is in the term's extension and is common to no other elements. The alkali metals are particularly reactive, having much lower ionization energies than their counterparts in other periods of the table, and they tend to form strong ionic bonds rather than covalent ones. These similarities in reactive properties mean that many of the alkalis can be exchanged with one another in the laboratory, which makes the higher-level chemical kind term "alkali metal" an important one to have on hand. The reactive similarities are explicated in terms of similarities in electronic configuration, a monadic CMP of the elements composing the higher-level kind.

This is just one of many examples of microstructural explication of higher-level kinds in chemistry based on reactive properties; each period of the table has a similar story to tell. In section 5.3, I return to considerations of higher-level chemical kinds in the discussion of the classification of water, but before I can do that a more detailed account of the relationship between microstructure and reactivity is needed.

4. Microstructure Grounds Reactivity. The previous section established that CMPs can be correlated with reactivity if and only if molecular-geometric properties are included as part of chemical microstructure. The task now is to determine the relationship between chemical microstructure and reactive behavior. I approach this task in two ways. In this section, I argue that microstructure is an explanans of reactivity in chemistry, and as such it can be used to ground, explain, or justify the individuation of chemical kinds according to ASCR. Importantly, reactivity is not used to explain microstructure—white phosphorus is not tetrahedral because it is more reactive than violet phosphorus; it is more reactive because it is tetrahedral. So this explanatory, grounding relationship is asymmetric. Observations about differences in reactivity can lead to inferences about microstructural change, but this pattern of reasoning still supports the idea that reactivity is explained in terms of or grounded by microstructure, because the explanandum in such cases is still reactivity and the explanans is still microstructure.

Note that the claim here is not that all changes in reactivity have presently been explained in terms of changes in microstructure, nor that microstructure causes reactivity, nor that there is a one-to-one mapping between every

reactive property and a parallel microstructural property. The explanatory relationship I am advocating is more modest. My claim is simply that microstructure often explains reactivity and that, when it does so, microstructure can provide additional explanatory information about the individuation of chemical kinds. Specifically, appealing to microstructural properties can reveal relationships among chemical kinds, such as shared outer-shell electronic structure, that explain similarities in reactivity and that are often not predictable from macroscopic observations alone. So the upshot of using microstructure to explain reactivity is that the resulting theory of chemical kinds can not only individuate single reliably repeatable reactions, but it can also both identify and explain similarities and differences among groups of reaction types.

In order for a chemical reaction to occur, chemical bonds must break, form, or both. The breaking and formation of chemical bonds is a microstructural process, and often it affects both monadic and relational microstructural properties of the substances involved in the reaction. While chemical reactions often display observable changes between the initial and final states of the system of substances involved in the reaction, these changes are always going to be associated with changes in the system's microstructure.

To elaborate: chemical reactions can be classified in a number of different ways, but each classification scheme implicitly or explicitly refers to the behavior of chemical bonds over the course of the reaction. For instance, one classification scheme divides chemical reactions into endothermic or exothermic reactions. The former requires the input of energy to occur and the latter outputs energy during its occurrence. Energy is a necessary component of the formation or dissolution of chemical bonds. In endothermic reactions, input energy raises energetic states of certain electrons involved in a bond, which increases the likelihood of the bond breaking and a different bond (with a different atom) forming. In exothermic reactions, energy is output as a result of atoms seeking lower-energy bonds than the ones in which they were originally participating.

The molecular geometry of the system changes during a chemical reaction. For example, when copper sulfate and sodium hydroxide are mixed, they react to form copper hydroxide and sodium sulfate. The four substances have distinct compositional formulas; thus they have distinct relational CMPs. In order, the substances are $CuSO_4$, NaOH, $Cu(OH)_2$, and Na_2SO_4. The reaction can be described in terms of observable changes—white flakes drop into blue liquid, and as the flakes dissolve a blue gelatinous solid forms—but these observable changes are precisely correlated with measurable changes in the microstructure of the system. Without changes in microstructure, there would be no occurrence of a reaction whatsoever.

Further, as shown by the phosphorus example in the previous section, differences in molecular-geometric microstructure from one substance to

the next, even if the substances have identical compositions, indicate differences in reactivity. By revisiting the phosphorus example, we can see further how differences in molecular-geometric microstructure can also determine or explain differences in reactivity. Recall that white phosphorus is composed of four-membered tetrahedral molecules, whereas violet phosphorus is composed of many-membered crystal structures. There is a difference in bond strength between the two. This difference in bond strength is a result of different molecular geometries, because as nuclei get closer together or farther apart, the bonds that hold them become more or less likely to break. The factors affecting bond strength are internuclear distance, number of electrons participating in a bond, number of nonparticipating electrons in the system, and distance between the participating nuclei and other nonparticipating nuclei present in the system—all chemical microstructural properties, most of which are molecular-geometric.

Analyzing bond strength reveals that white phosphorus is composed of smaller molecules with weaker bonds than violet phosphorus, and thus it is easier to break off an atom from a white phosphorus molecule. This breaking-off has to occur for phosphorus to react with oxygen to combust or with benzene or sulfur monochloride to dissolve. The stronger bond structure of violet phosphorus prevents such a breaking-off from occurring.

This discussion illustrates what I mean by 'changes in microstructure ground changes in reactivity', namely, that microstructural changes are necessary for changes in reactivity and are often used as explanantia for changes in reactivity. And not only can CMPs explain the reactivity of individual kinds, but they can also be used to pick out and explain patterns of reactivity among higher-level chemical kinds such as the alkali metals. To disprove the necessity of microstructural change for change in reactivity, one would need to show that a change in reactivity could occur without a change in any CMP. But because contemporary chemistry has shown that chemical reactions are, at a microstructural level, the breaking and formation of bonds, any change in a reaction is going to come with a change in molecular geometry and, thus, a change in a CMP. In the next section, I address some examples of chemical kind individuation that other philosophers have used to critique microstructural accounts of individuation. Using my more inclusive notion of CMP, I show how each of these supposedly problematic cases can be understood in microstructural terms and discuss why it is useful to understand them in this way.

5. Responses to Critiques of Chemical Microstructure. Here I survey a few of the more prominent case studies that have been used in the past as critiques of the microstructural approach to chemical kind individuation. I emphasize where the addition of molecular-geometric properties to the class of CMPs plays a key role in saving chemical microstructure, in order to underscore the importance of molecular-geometric properties to chemical

kind individuation. I begin with LaPorte's example of topaz and ruby; then I discuss his example of diamond. Finally, I address the problematic case of water, which Needham and others have used to argue against a microstructural approach to individuating chemical kinds.

5.1. Topaz and Ruby. LaPorte (1996, 122–24; 2004, 100–102) uses the examples of topaz and ruby to argue for two claims: first, that the extensions of chemical kind terms are chosen, rather than discovered, and second, that extensions of chemical kind terms do not always map onto differences in microstructure. While I do not contest LaPorte's first claim, a closer look at this pair of examples shows that the second is unfounded, because microstructure plays a key role in differentiating the chemical kinds in question. LaPorte argues that the extension of the term "topaz" includes all and only examples of a particular mineral kind, whereas the extension of the term "ruby" includes some but not all examples of a different mineral kind. I demonstrate that both terms refer to particular chemical microstructures, but whereas "topaz" refers to all minerals of a particular compositional formula, "ruby" refers to just one subclass of minerals of a particular compositional formula. Both kinds can be characterized in terms of CMPs.

The term "topaz" was coined before the advent of modern crystallography and was used to signify a brilliant yellow-orange gemstone. After von Laue and Ewald developed X-ray crystallography in 1912, Leonhardt published the first Laue photographs of topaz in 1924, determining its basic chemical composition, $Al_2SiO_4(F,OH)_2$. Around the same time, it was recognized that crystals with the same basic chemical composition and the same orthorhombic crystal structure were found in colors besides yellow-orange—as early as 1901 reports from Brazil came back describing rose and blue "topaz" (Derby 1901, 25). Differences in the colors of the minerals were due to minor aberrations in the crystal structure due to increased levels of iron, hydroxide, or chromium deposits. Scientists and other language users determined that the crystals of other colors were part of the extension of the term "topaz."

The term "ruby" was also coined before the advent of crystallography and was used to signify a brilliant red gemstone. When its chemical composition was investigated, it was found that ruby's basic chemical composition is Al_2O_3. Around the same time, it was recognized that crystals with the same basic chemical composition and the same hexagonal crystal structure were found in colors besides red, including blue, yellow, and pink. Differences in the colors of the minerals were explained in terms of differences in the presence of small deposits of chromium, titanium, iron, or some combination thereof. Scientists and other language users determined that crystals of other colors were not part of the extension of the term "ruby."

LaPorte reports the different determinations of extension as an exemplary case of choice among alternative possible extensions and against

microstructural essentialism, for, as he explains, the microstructural essentialist should be committed to saying that all colors of Al_2O_3 are ruby in the same way that all colors of $Al_2SiO_4(F,OH)_2$ are topaz—and history did not say that, although it could have. He writes, "Did we discover that, while ruby must be red, topaz need not be yellow? It seems not. It seems we could as well have concluded otherwise. Before the microstructure of topaz was explored, people knew that they used 'topaz' to refer to minerals of the same kind as the yellow ones they had picked out. But whether yellowness was a defining criterion of 'topaz' was, I think, not worked out. . . . That 'topaz' refers to all of one chemical compound and 'ruby' to only the red of another seems to represent decision, not discovery" (LaPorte 1996, 122–23).

Although LaPorte is right to conclude that the disanalogy between the two cases counts against microstructural essentialism, the case can still be made clearer if considered in microstructural terms. One interesting consequence of LaPorte's view is that while he has no problem deeming topaz a natural kind, he is initially ambivalent about the status of ruby and eventually decides it is not a natural kind. This differential treatment of the two terms, and the classes of objects they pick out, represents a fundamental difference between my own view and LaPorte's: I view both ruby and topaz as equally legitimate chemical kinds, but simply kinds that pick out relations at different levels of fundamentality. In other words, ruby is simply a lower-level chemical kind than topaz.

LaPorte's diagnosis of the present situation, namely, that "topaz" refers to all colors of $Al_2SiO_4(F,OH)_2$ where "ruby" refers only to red variants of Al_2O_3, is correct; this is how the terms are in fact used today. But the buck simply does not stop there, because color variation in these and all crystals is not a matter of unprincipled chance. Rather, color variation is the result of the presence or absence of a few nuclei of additional elements or of aberrations in internuclear distances in the crystal structure.

For instance, the brilliant red of rubies is due to the presence of chromium instead of aluminum in a few of the aluminum bond sites (and the more chromium, the redder the ruby). The general class of Al_2O_3 crystals, with chromium aberrations or without, is known as "corundum." The general class might have all been called "ruby," but it was not. Rather, the presence and quantity of chromium nuclei replacing aluminum nuclei determines the redness of a piece of corundum, and when chromium is present, the corundum is part of the extension of "ruby." This variation has different reactive properties than nonchromiated samples of corundum, because if the aluminum and oxygen in the sample were dissolved, chromium would precipitate out from the samples of ruby and not from the other samples.

Systematic explanations for the existence and intensity of different color variations in topaz can also be given in terms of CMPs. Blue topaz, for instance, obtains its color from slight aberrations in the internuclear distance

between some of the aluminum and silicon bond sites. This measure of internuclear distance is a molecular-geometric property of the sample. The further division of the classes of topaz and corundum into color-dependent subclasses thus turns out to be microstructural. The color range of topaz, as well as that of corundum, is a result of differences in molecular geometry from one sample to the next, whereas the difference between topaz and corundum is a difference in compositional formula. But both kinds of variation are due to relational CMPs.

So ruby, as the chromiated subclass of corundum, is an individuable mineral kind, as is topaz. The terms apply to two different levels of their respective taxonomies, with "topaz" occupying a place more similar to "alkali metal" and "ruby" one more similar to "sodium." Regardless of whether one believes that the extensions of these and other chemical kind terms are chosen or discovered, this example demonstrates that the extensions do map onto differences in chemical microstructure.

5.2. Diamond. LaPorte's (2004, 101) study of diamond illustrates the need for molecular-geometric properties in the class of CMPs. LaPorte compares diamond with its allotrope, charcoal, and claims that the microstructure of the two substances is identical. From this he concludes that microstructure cannot determine the extension of these chemical kind terms. LaPorte introduces the example with a historical tale about when it was realized that diamond and charcoal have "exactly the same" chemical composition as one another. In the same paragraph he also asserts that the "chemical structure" of the two substances is identical. While the former is true, the latter is not; the two allotropes are made up (as all allotropes are) of atoms of the same element arranged in different molecular geometries.

Diamond and charcoal are allotropes of carbon, in the same way that white and violet phosphorus are allotropes of phosphorus. Both diamond and charcoal are composed solely of carbon nuclei but with different spatial arrangements between the nuclei—in charcoal, an amorphous collection of nuclei assembles itself with irregular internuclear distances, molecule sizes, and bond lengths, whereas in diamond the nuclei are arranged in a rigid, face-centered-cubic crystal lattice.

Here LaPorte is correct to characterize diamond and charcoal as having identical chemical composition. He recognized that the naive view of relational CMPs, the one in which nothing besides compositional formula matters, would identify both substances as microstructurally identical. But if one thing is to be taken away from this essay, it is this: compositional formula is not the only microstructural feature of groups of atoms that counts for chemical classification, for chemical reactivity, or for a sophisticated view of chemical kinds. Molecular geometry matters, and in this case, as in the case of phosphorus, molecular geometry is the only CMP that can be used to distinguish one substance from the other.

5.3. Water. The relationship between water's identity and its microstructure has long been a matter of debate among philosophers of science. The debate centers around responses to Putnam's "Twin Earth" intuition pump (1975, 139–43), which argues that if a substance with all the observable properties of water but without the chemical formula H_2O were found on another planet, it would be inappropriate to call this substance "water." Putnam used the Twin Earth story to argue for his version of microstructural essentialism, and both the example and the view have come under attack from a number of directions. Recently, many philosophers of chemistry have argued that microstructure cannot individuate water,[7] with only a resolute few defending some variant of microstructural individuation (see, e.g., Hendry 2006). The argument against microstructural conceptions of water has founded most contemporary chemical attacks on microstructural essentialism, and here I offer one option to begin dissolving the debate.

This discussion should be prefaced by pointing out that few philosophers of chemistry disagree on the chemical, physical, and biological properties of water, and much attentive work has been done in philosophy of chemistry to rectify Putnam's naive conception of water's structure. In its liquid phase, water is a complex and dynamic collection of chemical species including H_2O, OH^-, H_3O^+, and so on, along with elaborate networks of hydrogen-bonded chains of ions and normally distributed isotopic variation among both hydrogen and oxygen atoms. Water has definite physical properties, such as a molar mass of 18.015 g/mol, a density of 1 g/cm^3 under atmospheric pressure, a melting point of 0°C and a boiling point of 100°C, as well as the ability to conduct electricity and dissolve a wide variety of solutes. In its solid phase, water (ice) forms a hexagonal crystal lattice under normal conditions, although nonhexagonal crystals of H_2O, known as clathrate hydrates, have been observed both in laboratories and in geological formations. Water is one of the few substances whose solid phase is less dense (by about 8%) than its liquid phase. Water slakes thirst and supports life on this planet. Likewise, few philosophers of chemistry disagree on the chemical and physical properties of the H_2O molecule. It is polar, has a bent or "Mickey Mouse" geometry with an average bond angle of 104.5° and average O–H bond length of 0.96 Å. The source of disagreement is about what to do with all this information when it comes to the classification of water as a chemical kind.

Needham and Van Brakel have developed the most extensive anti-essentialist responses to the Twin Earth problem. Van Brakel formulates the objection particularly clearly:

7. Compare, e.g., Needham (2000, 2011), Van Brakel (2000), Weisberg (2006), VandeWall (2007), and Chang (2012).

> What does it mean to say that water consists of molecules "made up of just three atoms, two atoms of hydrogen and one of oxygen." Underlying microscopic essences vary as much with context or circumstance as the nominal essences. There are H_3O^+ and OH^- ions in liquid water. There are H_4O_2-molecules, as well as other H_2O-polymers in water vapour. And how much ionisation or dimerisations and polymerization there is, depends on the temperature and other contextual variables. The pragmatic answer that water is *predominantly* H_2O is not sufficient if we are looking for essences. (Van Brakel 2000, 80, emphasis in original)

In other words, because water is made up of a much wider variety of chemical species than simply H_2O molecules, the molecule H_2O cannot be identified with water. Needham has developed this objection into a detailed, historically informed, and macroscopically oriented account of the extension of the term "water," as illustrated by this excerpt:

> Water in particular is an inorganic substance which, as mentioned [earlier], is not molecular, except under certain conditions in the gas phase. It comprises so many different kinds of entities of varying longevities in the liquid phase that if distinctness of kinds of microparticles were the guide to distinctness of substances, water would be a mixture. But as outlined [earlier] (and described in more detail in Needham 2000 and 2002), this is not the guide. Rather, macroscopic criteria determine that a quantity of matter whose microstructure scientists investigate is in fact water. Hendry (2006, p. 872), in a much weakened and better informed version of the microstructuralist thesis along the lines of that at issue in this section, claims that "water is the substance formed by bringing together H_2O molecules and allowing them to interact spontaneously". But this is just to say that the molecular character of the gas phase at low pressure disappears on condensation; it doesn't actually give the microstructure of liquid water. (Needham 2011, 16)

Needham concludes with a more overtly anti-essentialist perspective, "It is therefore necessary that what is water is a single substance with the characteristic features it in fact has. What is water is, of course, what the 'water' predicate applies to, and as with any singular term, whatever identities it is involved in are necessary. Water's having its characteristic features necessarily is nothing to do with this" (Needham 2011, 20).

What Needham has done, then, with the available information about water and H_2O, is to craft an argument for macroscopic individuation and against microstructural essentialism. Van Brakel, likewise, concludes that the essence of water cannot be H_2O. But while these critiques are sound ones against microstructural essentialism, they largely overlook the fact that there is still a relationship between water and H_2O, as well as between "water" and "H_2O," that is regularly mentioned and used in chemical re-

search and pedagogy. This relationship is complicated, because water is not a mere aggregate of H_2O molecules, but it is nonetheless a fact that water is made up of hydrogen and oxygen in a 2:1 ratio, and an account of chemical individuation should be able not only to accommodate this fact but to use it to construct explanations, predictions, and other inferences.

The account I have developed in this essay, wherein reactivity individuates chemical kinds and microstructure grounds that individuation, accomplishes both these tasks. Rather than playing down the connection between water and H_2O, my account can be used to ground the reactive properties of water in its microstructure without committing to the naive water-as-H_2O-aggregates view. I have discussed my expanded definition of chemical microstructure properties at some length, showing that chemical microstructure encompasses a variety of property types, including monadic properties of atoms, compositional ratios, and molecular geometry. And I have demonstrated that chemical microstructural properties can explain not only fundamental chemical kinds for which the ASCR criterion holds but also higher-level relations among chemical kinds, such as the grouping of alkali metals and the varieties of topaz. I have also pointed out that there need not be a one-to-one mapping between reactive properties and microstructural properties in order for explanatory relationships of this sort to hold.

Taken together, these points form the basis of a new account of water's relationship to H_2O: water may be individuated according to ASCR, and it is important to note that subspecies of water, such as deuterium oxide, and colloquial referents of "water," such as seawater, will not enter into all the same chemical reactions as plain water itself. With water so individuated, a story can be told about its microstructure to explain its reactive properties and ground its relation to H_2O. Water dissolves solutes because of the polarity of H_2O molecules, as well as the various ionic species and hydrogen-bonded networks that reside within it. Nonetheless, chemical reactions in water can be predicted and explained via chemical equations referring to H_2O because the compositional ratio of 2H:1O holds of macroscopic samples of water, despite variation in molecular and ionic species.

Water is not a foundational (i.e., infimic) chemical kind under the account I have laid out here—nor should it be, because "any old water" is not a chemically useful reagent; instead, specific kinds of water (e.g., distilled, deionized, heavy, superheavy, etc.) are. Still, under this account it is still possible to describe a panoply of relationships between aqueous substances and varieties of H_2O molecules, H^+ and OH^- ions, and additions or subtractions of deuterium. The account allows for the conclusion that water does not map onto a single molecular geometry, but that nonetheless the 2H:1O compositional ratio holds of it. Finer-grained accounts of the molecular geometry of water are sometimes useful in chemical predictions and explanations, and other times the coarser-grained compositional ratio proves the more

fruitful microstructural explanation of water's reactive properties. In either case, one may remain silent on the question of whether water has an essence, and if so, what it might be. The fact that this silence frustrates some theories of reference seems a larger problem for those theories than for this account, which preserves the inferential structure and collected knowledge of chemistry.

6. Conclusions. I have developed an account of chemical individuation in which chemical kinds are individuated according to their reactivity, and their reactive properties are in turn explained in terms of changes in microstructure. This account is meant to reconcile recent insights from the philosophy of chemistry about the failure of microstructural essentialism with the strong presence of microstructural explanation and reference to microstructure in modern chemistry. I argued that chemical identity is obtained when two samples enter into all and only the same chemical reactions and that looking to microstructure can not only explain many cases of chemical identity, but it can also rationalize observed similarities and differences between chemical kinds and justify the grouping of chemical kinds into higher taxa.

My account relies on an expanded conception of chemical microstructure, which calls attention to the existence of both monadic and relational chemical microstructural properties, as well as to molecular geometry as a kind of relational chemical microstructural property. I used this conception of chemical microstructure to show how changes in microstructure ground changes in reactivity, and I applied my account to three prominent examples in the philosophy of chemistry literature. I showed how in the cases of topaz and ruby, diamond, and water, reactivity is sufficient to pick out each of the relevant chemical kinds and how in each case differences in microstructure explained differences in reactivity.

Underlying this account is a pragmatic view of chemical classification, wherein the purpose of individuating chemical kinds is to be able to use the right words to accomplish chemical projects such as explanation, prediction, and synthesis. While this motivation is rather distant from Kripke's and Putnam's initial concerns about fixing reference through essences and the possibility of trans-world identity, the critical response from philosophers of chemistry to those initial concerns has raised more general questions about classification and kinds in chemistry. This account is meant to address those concerns and to show that discussions of chemical classification can be peacefully separated from essentialist interests.

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