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The Roles of Representations and Tools in the Chemistry Laboratory and Their Implications for Chemistry Learning

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In this historical and observational study, we describe how scientists use representations and tools in the chemistry laboratory, and we derive implications from these findings for the design of educational environments. In our observations we found that chemists use representations and tools to mediate between the physical substances that they study and the aperceptual chemical entities and processes that underlie and account for the material qualities of these physical substances. There are 2 important, interrelated aspects of this mediational process: the material and the social. The 1st emphasizes the surface features of both physical phenomena and symbolic representations, features that can be perceived and manipulated. The 2nd underscores

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the inherently semiotic, rhetorical process whereby chemists claim that representations stand for unseen entities and processes. In elaborating on our analyses, we

- Examine the historical origins and contemporary practices of representation use in one particular domain—chemistry—to look at how developments in the design of representations advance the development of a scientific community, as well as the understanding of scientists engaged in laboratory practice.
- Examine representations spontaneously generated by chemists, as well as those generated by their tools or instruments, and look at how scientists—individually and collaboratively—coordinate these 2 types of representations with the material substances of their investigations to understand the structures and processes that underlie them.
- Draw implications from the study of scientists to make recommendations for the design of learning environments and symbol systems that can support the use of representations by students to understand the structures and processes that underlie their scientific investigations and to engage them in the practices of knowledge-building communities.

> In an important sense, chemistry is the skillful study of symbolic transformations applied to graphic objects. (Hoffmann & Laszlo, 1991, p.11)

How do scientific representations and tools contribute to the investigation and understanding of physical phenomena? How do scientists use these resources to penetrate the surface characteristics of phenomena, so as to understand underlying structures and processes that account for these surface features? What are the features of representations that allow them to do this? What implications do the answers to these questions have for educational practice? This historical and observational study describes how scientists use representations and tools in the chemistry laboratory to observe, understand, and manipulate molecules; these are the chemical entities that underlie and account for the material qualities of physical substances.

In the history and current practice of chemistry, understanding molecular properties and processes has been a challenge, in large part because molecules and their properties are not available to direct perception. Consequently, chemists have designed tools and representational systems that mediate between something that they can not see and something that they can. Within a community of shared goals, knowledge, and discourse, chemists use representations and tools to explain, predict, and change the chemical phenomena that are the focus of their work. There are two important, interrelated aspects of this situated, mediational process: the material and the social (Brown, Collins, & Duguid, 1989; Greeno, 1998; Wertsch, 1985, 1991). The first emphasizes the surface features of both physical phenomena and symbolic representations, features that can be perceived and manipulated. The second underscores the inherently semiotic, rhetorical process whereby chemists

claim that representations stand for unseen entities and processes. Once this relation is established, scientists can reason with the physical features of representations to make inferences about phenomena that are insufficiently explained using their surface features alone.

This study provides details about the discourse practices of scientists and how they use language, representations, and tools within the material and social context of their laboratories. Our findings suggest that scientists use these resources in their investigations to

- Express their research goals in terms of the molecular structure of compounds they intend to create.
- Reason about the physical processes needed to synthesize these compounds.
- Verify the underlying composition and structure of the synthesized compounds.
- Convince the scientific community that the compound they synthesized is the one they intended.
- Confirm their membership in the scientific community.

The findings of this study have implications for how students can come to have a deeper understanding of science. Educational researchers (Brown & Campione, 1994; Scardamalia & Bereiter, 1994a) have used the inquiry and discourse practices of scientific communities as models for the design of communities of students who are similarly engaged in shared knowledge building. However, scientific discourse practices have been used primarily as a rhetorical metaphor to advance the importance of discourse in the classroom activities of students.

In this study, we go beyond scientific discourse as metaphor to examine the details of these practices and derive specific implications for the ways students may come to understand science through inquiry, discourse, and representation use. We discuss the implications that our findings have for the use of language, representations, and tools by teachers and students in the context of laboratory investigations (Krajcik et al., 1998). Specifically, we describe how teachers and students can use these resources to

- Express their understanding of observed phenomena in terms of underlying, aperceptual entities and processes.
- Test their understanding with experiments on physical materials.
- Create a knowledge-building community around the common use of representations and tools to investigate and explain chemical phenomena.

Scardamalia and Bereiter (1994a, 1994b) and Brown and Campione (1994; Campione, Brown, & Jay, 1993) suggested that technology can support knowl-

edge-building communities by providing students with tools to search and organize information, write reports, and communicate with others. Other researchers (Kozma, in press; Pea, 1992, 1994; Roschelle, 1992) have demonstrated how technology can provide students with symbolic representations of scientific phenomena that they use as props to support their learning conversations. We extend this notion in our discussion of educational implications to recommend the design of technology-based representational environments and symbol systems that

- Provide students with an expressive medium in which the features of representations structure students' thinking about the entities and processes that underlie physical phenomena.
- Connect student-generated representations to tool-generated representations during investigations of physical phenomena.
- Scaffold and support students' use of representations to question, observe, describe, discuss, explain, and argue about chemical entities and processes within a knowledge-building community.

These representational environments can help students understand the underlying structures and processes of scientific phenomena, as well as the physical and social processes by which these structures are established.

REPRESENTATIONS IN SCIENTIFIC THINKING AND PRACTICE

Representations and Scientific Expertise

A long history of experimental research has established the fact that scientists and other experts are able to organize information into large, conceptually meaningful patterns (Glaser & Chi, 1988). Physicists, for example, look at a range of textbook problems and cluster them in ways that correspond to underlying concepts and principles of physics, such as "force" or "work energy," which they use in turn to solve problems (Chi, Feltovich, & Glaser, 1981; Larkin, 1983; Larkin, McDermott, Simon, & Simon, 1980). Representations play an important role in this process. An example of the role they play is demonstrated by the physicist in Larkin's study (1983, pp. 91–92) who began his work by drawing a diagram of the problem situation. Some of the symbolic elements of the diagram represented the objects and spatial arrangements mentioned in the problem statement and others (i.e., force vectors) corresponded to conceptual entities (i.e., Newtonian force) that were evoked from memory. The physicist reasoned with this representation, moving back and forth between the components of the constructed diagram and the requirements of the solution held in memory. When conflicts between the representation

and potential solution could not be resolved, he abandoned the diagram and created one that represented an alternative and ultimately successful solution. Finally, he used a mathematical equation that corresponded to the solution to produce the appropriate numerical answer.

In our own research with experts in chemistry (Kozma & Russell, 1997), we found that the patterns they create are both based on and distinct from the symbolic forms used to represent phenomena. In one task, experts examined chemical phenomena expressed in a variety of ways (e.g., graphs, molecular animations, equations, and video segments of experiments). As in the studies of physicists, chemists were able to create large, chemically meaningful clusters that they described using conceptual terms (e.g., *gas law* and *collision theory*). At the core of these clusters were common, same-medium pairs of representations (e.g., two different graphs of the same phenomenon). However, the experts were distinguished from novices by the fact that their clusters were much larger and consisted of multiple representational forms (e.g., graphs, animations, etc.). In a second task, chemists were asked to view a chemical phenomenon expressed in one representational form and transform it into another (e.g., transform a chemical equation into a corresponding graph, select an animation that corresponded to a lab bench experiment, etc.). In general, chemists were able to transform any given representation into chemically meaningful representations in other forms.

These studies demonstrate that expert scientists have significant representational skills and competencies. They use their knowledge of the domain, their representational skills and the features of representations to create theoretically based groupings of problem situations and to reason about their solution.

Representations and Scientific Practice

Although studies of expertise provide us with insight into the skills and knowledge of scientists, they do not provide us with an understanding of the processes by which scientists come to know, within the context of their laboratory investigations. Observational studies often capture the social–material nature of representation use that is missing in experimental studies of expertise (Dunbar, 1997). These studies document that the use of representational skills is an important component of scientific investigation and knowledge creation.

For example, Woolgar (1990) studied scientists as they examined the structural changes that amorphous alloys undergo in the course of heating. These changes are not observed directly but are monitored by reference to more measurable property changes, such as changes in electrical resistance, which are revealed by instrument-generated representations, such a trace on a pen-chart recorder. Woolgar described the activity of scientists in which they observed the recorder as the line it generated forms a downward slope. He analyzed their discourse as they observed

the shape of the emerging graph, expressed surprise at the results, and compared the shape of the graph with those from previous experiments as they attempted to explain their observations. Woolgar's example illustrates that a representation's meaning is not straightforward but hinges on features of the representation (in this case, its slope), the features that scientists expect to see, and comparisons of features across representations from several experiments.

As the Woolgar (1990) study suggests, the meaning of a representation is often generated by coordinating features within and across multiple representations. Goodwin (1995) described how an oceanographic research team uses representations generated by a cluster of instruments lowered into the sea to collect a variety of data on water characteristics. The data were presented on various displays in the on-board laboratory and interpreted by scientists of various disciplines (physical oceanographers, geochemists, and biologists). In understanding the data, Goodwin observed scientists as they mapped the features of a representation (e.g., the peak of a graph) onto other features within the visual field (e.g., the relation between one peak and others) and onto features of the frame of reference (e.g., relation between the peak and numbers on the indexical scale). He also observed scientists coordinating representations of the same phenomenon generated by different instruments. In this study, scientists also coordinated features across representations generated by various tools (e.g., a conductivity, temperature and depth sensor and a precision depth recorder) to assign meaning to the data and co-construct a shared understanding of the seawater characteristics that they were studying.

Scientists do not necessarily concur as they collaborate to construct meaning from representations. Amman and Knorr Cetina (1990) illustrated the rhetorical nature of this process in their study of geneticists. They described how scientists gathered together to analyze visual traces on recently exposed X-ray film that were generated by radioactively marked DNA and RNA fragments separated in an electrophoresis gel. Their interaction was organized as conversational turns sequentially structured as a pattern of adjacent question–answer pairs that were accompanied by deictic statements and gestures to specific features of the representation. As they examined the film they pointed, made verbal references to marks on the film, drew inferences, raised objections, asked questions, returned to the film, provided replies, and so on, until a conclusion—not necessarily consensus—was reached.

These studies illustrate the processes by which scientists use representations to understand scientific phenomena. They also demonstrate the inherently social nature of representational practice.

Representations in the Science Classroom

Educational researchers are beginning to see the importance of representational practice in the science classroom. For example, Roth and McGinn (1998) advo-

cated the use of representations of scientific phenomena within the context of student discourse and scientific investigation. Like scientists, students engage in research and use representations in a rhetorical context to talk about their investigations. In the course of these interactions, students appropriate both the use and meaning of representations.

A study by Roschelle (1992) showed how this can happen. In this study, two students used a representational environment, *Envisioning Machine*, to explore the concepts of velocity and acceleration. With this environment, a thrown ball was represented in two different spaces on a computer screen. In one space, it was represented as a black circle and this object behaved over time as would a thrown ball. In the second space, the ball was represented by a white circle and changing arrows (i.e., vectors) that corresponded to the velocity and the acceleration of the ball as it traversed its trajectory. Students altered the vectors on the white ball to match the motion of the black ball. In doing so, the students negotiated a shared understanding of acceleration through a series of interleaved assertions, gestures, actions, requests for clarification, acknowledgments, elaborations, and other linguistic devices for signaling agreement and fixing troubles in shared understanding. During discourse, students referenced the representations by gaze, pointing, and other means, as a way of supporting the conversation and meaning negotiation. Through these deictic references and cross-references to their surface features, the representations were used as rhetorical devices that advanced shared understanding.

Similarly, in a study from our laboratory (Kozma, in press) chemistry students used a representational environment called *4M:Chem* (Russell et al., 1997) to understand chemical equilibrium. In their discourse, students coordinated the features of a graph with those of a video of the experiment to argue that equilibrium between two reagents occurred when the slopes of partial pressure in the graph were at zero rather than when they crossed, as they had both previously believed. By using representations in this rhetorical way, the students' understanding of both equilibrium and the representation changed.

These studies demonstrate the role that representations can play in supporting the discourse of students as they explore scientific concepts and principles. During their conversations, students draw on specific features of representations to support their convergent understanding.

GOALS OF THIS STUDY

This literature review documents the important role that representations play in scientific understanding and practice and the role they can play in science learning. With this study, we contribute to the aforementioned literature in three ways:

- We examine the historical origins and contemporary practices of representation use in one particular domain—chemistry—to look at how developments in the

design of representations advance the development of a scientific community, as well as the understanding of scientists engaged in laboratory practice.

- We examine representations spontaneously generated by chemists, as well as those generated by their tools or instruments, and look at how scientists—individually and collaboratively—coordinate these two types of representations with the material substances of their investigations to understand the structures and processes that underlie them.
- We draw implications from the study of scientists to make recommendations for the design of learning environments and symbol systems that can support the use of representations by students to understand the structures and processes that underlie their scientific investigations and to engage them in the practices of knowledge-building communities.

LANGUAGE, ACTIVITY, AND COMMUNITY IN CHEMICAL HISTORY

In addition to observational methodologies, historiography has been used to shed light on the ways scientists come to know and understand within social–material contexts (Kuhn, 1962). Only recently has this methodology been used as a way of gaining insight into contemporary practice and deriving implications for education (Cole & Engeström, 1993), particularly as these relate to the use of representations (Kaput, 1994). We extend this work to consider historical changes in the use of scientific representations in chemistry and the implications these have for educational environments and activities. We find that the design of new representations afforded new activities and new ways of thinking about chemistry, primarily because of particular features embedded in their structure, as described below. These advances in representations advance the knowledge development in both the discipline and individuals that practice it (Luria, 1981; Vygotsky, 1962, 1978). In the concluding section in this article, we derive recommendations about the design of new representational environments that can support chemical understanding and representational competence among students.

We begin our historical investigation by examining changes in the late 18th century as chemistry moved from an understanding based on the perceptually accessible physical qualities of substances to one based on their aperceptual, elemental composition. This shift in understanding was both enabled and shaped by a set of corollary changes that included the formation of a new chemical terminology or nomenclature, a new set of tools, the restructuring of chemical activity, and a redefinition of the chemistry community. These early developments continue to influence chemical practice to this day in what Cole and Engeström (1993) called "history in the present."

Before there was a science of chemistry, there existed a body of practical knowledge of materials based on crafts of the smith, the dyer, the glass maker, the distiller, and several others (Crosland, 1962). This technical knowledge, together with some ideas from alchemy (itself part technical and part philosophical), formed the early beginnings of chemistry. This practical knowledge was based on the surface features of physical substances, as denoted by the names they were given. In his history of the language of chemistry, Crosland (1962) showed that, prior to the 18th century, the names of substances were derived primarily from physical qualities, such as color, taste, smell, and consistency. These surface features were useful in making rudimentary distinctions among substances. Color was the most commonly used feature and this practice goes back to ancient times when Egyptians used the word *hetch,* or *white*, for silver and *vatch,* or *green*, for malachite and other green ores of copper. Crosland speculated that the use of color and other physical characteristics were of particular importance to craftsmen, who valued rudimentary chemical knowledge as an aid to the preparation of materials essential to their trade. The purpose of these craftsmen was to produce artifacts (jewelry, clothing, glass, etc.) for which color and other material qualities were important considerations.

The late 18th century is commonly recognized as the time when chemistry became a modern science (Brock, 1992; Partington, 1989). It was during this period that a group of French chemists led by Antoine Lavoisier set into motion a series of changes that reformed chemical nomenclature, established new norms for scientific investigation, and standardized structures for scientific argument that contributed to the development of the discipline of chemistry (Anderson, 1984). Chemistry was also given a new purpose. For Lavoisier, the purpose of chemistry in the 18th century was " subjecting different bodies in nature to experiment … [so as to] decompose them and … examine separately the different substances that enter into combination" (as cited in Anderson, 1984, p. 136).

By the 18th century, the nomenclature that evolved over the centuries for one set of purposes collided with this new purpose, and the limitations in the nomenclature became obvious. By this time, the number of substances that scientists were able to isolate had grown dramatically. Names based on color, smell, and other surface properties were no longer sufficient to discriminate among these substances; many substances had the same color as others or had no color at all. These terms were also not useful in facilitating the analysis of underlying composition.

The growth in chemical research and the recognition of the limitations of chemical nomenclature occurred within the philosophical context of the French Enlightenment (Anderson, 1984). Lavoisier and his colleagues were very much influenced by this philosophical orientation, particularly as it was expressed by Etienne Bonnot Condillac. For Condillac, the relation between language and thinking was integral. Condillac contended that symbol systems enabled thinking: "Analysis is only performed, and can only be performed, using signs" (as cited in

Anderson, 1984, p. 162). Conversely, thinking was also constrained by the structure of the language: "We only reason well or reason badly in so far as our language is well or badly constructed" (as cited in Crosland, 1962, p. 171).

The challenge, then, for the 18th century chemists was to go beyond the acknowledged deficiencies of the nomenclature they inherited and design a new language that could be used for this new, emerging purpose: the classification of chemicals and the identification of their constituent components. The requirements of this new language were developed by Lavoisier, Guyton de Morveau, and several colleagues in a series of works, the most prominent being the *Méthode de Nomenclature Chimique*, published in 1787. Rather than a language based on physical properties, these authors believed the name of a compound would reflect the elemental components that account for its physical properties. Substances that could not be decomposed (i.e., elements) would form the basis of the entire nomenclature. Compound chemical structures would be named by compounding the words used for their elemental components. The use of compound terms gave a material reality to the underlying multiple elements.

In this way, the language was also to be structured such that operating on symbols would be analogous to operating on substances; that is, the composition or decomposition formed using terms would correspond to the results produced in the laboratory (Anderson, 1984). So, for example, the combination of hydrogen and oxygen would produce water and the chemical name for water would consequently be based on these compositional elements. Consequently, the new nomenclature influenced both the language and activity of chemists. The structure of the language would facilitate—indeed, require—the experimental decomposition of new chemicals in order for them to be named, and operations on the words helped chemists think about the operations that they employed in the laboratory.

It was explicit in Lavoisier's thinking that this restructured language would both restructure activity and the community that used the language. Building on the ideas of Condillac, Lavoisier stated that

> A well formed language, a language in which one will have captured the successive and natural order of ideas, will bring about a necessary and even prompt revolution in the manner of teaching. It will not allow those who profess chemistry to diverge from the march of nature. They will have either to reject the nomenclature, or else to follow irresistibly the route that it will have marked out. (as cited in Anderson, 1984, p. 176)

Thus, the nomenclature was not just a new set of names but embedded in its structure and use was both a new set of chemical activities and a new chemical community. The object of chemical activity shifted from the external to the internal, from the identification of material substances to the determination of their underlying composition. By embedding this focus into the very language of the field, Lavoisier institutionalized these new activities of analysis and decomposition and assured

that they would be carried on by others. By moving from a focus on the surface characteristics of physical substances to their underlying, aperceptual elemental composition, Lavoisier took a significant step down a new road that transformed the field of chemistry into that of a molecular science.

Decomposition and analysis were fruitful activities well into the 19th century and chemists were served well by the nomenclature of Lavoisier, but as chemists explored the composition of compounds and their elementary constituents, they came to know more about how these elements could be recombined into complex molecules. Since the early 20th century, synthesis—or the making of chemicals—has come to be "the contender with analysis for the heart of chemistry" (Hoffmann, 1995, p. 22). This development both drove and was enabled by the development of new representations. Words alone were insufficient to support chemists' thinking about the spatial arrangement of atoms that were needed to synthesize a specific molecule. A new representational system was needed with features that more closely corresponded to the structure of molecules. This system was the molecular structural diagram. Structural diagrams have become ubiquitous in chemistry, particularly organic chemistry, to the point where Ege (1989) contended that "Professional organic chemists cannot talk to each other without drawing structures" (p. 2). Chemists in our observational study used the features of these structural diagrams, along with scientific language, to think about the arrangement of atoms in the molecules they wanted to synthesize and the processes needed to achieve these products.

Our historical analysis documents that the design of representational systems is a key cultural activity that affects the composition of a community, the other activities in which its members are engaged, and the understanding that community members have about its domain of knowledge. This understanding is both enabled and constrained by symbolic features of the representational system and the operations that can be performed using it.

REPRESENTATIONS, TOOLS, AND DISCOURSE IN THE CHEMISTRY LABORATORY

The goal of our observational research is to understand how culturally derived activities and representational systems support the work of chemists in their laboratory and, ultimately, how they can support the learning of students. To this end, we observed and interacted with chemists as they were engaged in their laboratory work.

Methodology

Participating laboratories. Two different settings were chosen for our observational study. One was an academic laboratory, engaged in the synthesis of organic compounds. Although there are often clear industrial applications for these

compounds, the major purposes of this laboratory were basic science research and the training of graduate students in chemistry. The other setting was a pharmaceutical firm, which devotes most of its energies to the development of marketable drugs. Some basic research may result from drug development work, but the work itself was driven by the demand to create marketable products. There was some interaction between the university where the academic lab was located and the pharmaceutical firm. In fact, graduates from the university would occasionally obtain positions at the pharmaceutical firm.

Procedure. We gained access to both laboratories through contact with the laboratory directors. In the case of the academic lab, the director was a faculty member in the department of chemistry who directed several graduate students and postdoctoral fellows in his lab. We observed and interviewed three chemists in this lab—two graduate students early in their careers in graduate school and a postdoctoral fellow who had been with the lab group for about 2 years. We spent 1 full day in the lab with each of the students and the postdoctoral fellow. We also attended two problem sessions with the lab group: One session was devoted to presentations of recent lab work, whereas the other was spent discussing solutions to problems shown in the literature.

In the case of the pharmaceutical lab, contact was made with the vice president of research, who in turn identified six chemists who would work with us. All of the chemists in this lab were very experienced and had spent several years working either within this organization or at other laboratories. Their educational backgrounds varied, with some holding bachelor's degrees, some with master's degrees, and others with doctorates. Although most of the chemists at the pharmaceutical firm spent their time doing bench work, one of the chemists was a project director who spent much of his time directing other chemists in his lab. Some of these chemists interacted with each other during group meetings and at other times during the course of their work, whereas others never met because they worked in very different project groups.

Sixty-four hours were spent observing chemists working at the bench, attending group research or problem-solving meetings, and interviewing these chemists and their supervisors. The observations during laboratory work and interviews with the chemists were audiotaped. Field notes were written of all observations and some artifacts were collected from the academic lab, artifacts such as thin layer chromatography (TLC) plates, gas chromatography plots that would have otherwise been discarded, and public documents about the pharmaceutical firm. However, we were required to sign nondisclosure agreements with the pharmaceutical laboratory. As a result, no drawings were made of any of the chemical structures displayed at any of the meetings or in the notebooks we reviewed with the chemists at this company. This compromise with the reality of the proprietary setting limits our ability to reference these representations in the analyses of this re-

port. However, because our analyses depend on the relation between what chemists say and certain features of the representations that they use, we provide representations of similar chemical structures that can support the reader's understanding of our presentation.

The audiotapes for all of the observations and interviews were transcribed. From these transcriptions and field notes, we identified critical incidents in which representations and tools were used by chemists to accomplish their work. For these incidents, we examined the transcripts and features of the artifacts to determine how these supported chemists' attempts to understand specific problems they encountered in chemical synthesis. In reporting our evidence, we embed annotations in the verbal protocols of our subjects that identify references that they made to objects in their immediate context. This is a technique used in other observational studies (Amann & Knorr Cetina, 1990; Goodwin, 1995; Hall & Stevens, 1995; Ochs, Jacoby, & Gonzales, 1994; Roth & McGinn, 1998; Suchman & Trigg, 1993), although the specific format of the annotation varies somewhat across studies. These references allow us to examine the way participants coordinate their verbal activity with both symbolic and physical objects in their environment. Our analyses are divided into three considerations: (a) how scientists use diagrams to represent the structure of physical substance the synthesize, (b) how scientists use tool-generated empirical representations of structure, and (c) how scientists use discourse within the chemistry community to confirm underlying structure.

Diagrams and the Representation of Underlying Structure

The chemists we observed were all engaged in the process of chemical synthesis. As mentioned in our historical section, the synthesis of new compounds has now become a central goal for contemporary chemists. As Nobel laureate Hoffmann (1995) pointed out,

> Chemists make molecules. They do other things, to be sure—they study the properties of these molecules; they analyze as we have seen, they form theories as to why molecules are stable, why they have the shapes or colors that they do; they study mechanisms, trying to find out how molecules react. But at the heart of their science is the molecule that is made, either by a natural process or by a human being. (p. 95)

Whether motivated by finding a cure for Alzheimer's disease, a new fabric fiber, a nutritional additive, a low-emission fuel, or a high-insulation material, many contemporary chemists engage in the process of synthesizing new compounds. Reaction, separation, and identification are essential components of this process, but beyond the specification of elemental components, as Lavoisier envisioned, chemists engaged in synthesis must also determine the structure of the compound.

Two or more compounds may be composed of the same elements, but the elements may be arranged differently in these compounds. Those that have different arrangements are called *isomers*. Typically only one (if any) of these arrangements has the desired curative, nutritional, or insulative properties. Consequently, chemists must specify both the composition and the arrangement of elements that is desired. This activity required and was facilitated by a different representational form.

Structural diagrams have surface features that chemists can use to represent the arrangement of atoms in molecules and to reason through the ways to synthetically change their structure. An example of a structural diagram (not taken from our observations) is displayed in Figure 1 (a diagram of acetic acid, or CH_3CO_2H). There are three types of features that make structural diagrams useful in synthesis: (a) those that represent constituent components, (b) their relative arrangement in space, and (c) the bonding between them.

In the case of Figure 1, the letters represent the atoms and the lines represent both their bonds and their spatial arrangement. The diagram shows that the three hydrogens are in a pyramidal arrangement around the carbon to which they are each bonded. The solid wedge used to attach one of the hydrogen atoms to the carbon atom indicates that this hydrogen atom is coming out of the plane of the paper toward the viewer. The dashed bond to another hydrogen atom indicates that the atom is behind the plane of the paper. The single lines represent single electron pair bonds. The double lines between the carbon and one of the oxygens represents a double bond in which two pairs of electrons are shared. Chemists can assemble and manipulate these symbolic elements in ways that correspond to the structure of molecules and the processes that are used to synthesize them.

Diagrams and drawings of chemical structures were pervasive in our observations in both the academic and pharmaceutical laboratories. The centrality of these representations in chemistry work is reflected in the design of laboratory spaces in the facilities that we visited. Every lab devoted some space on the walls for white boards and chemists used these to draw structural diagrams of the chemicals that they worked with. In fact, the pharmaceutical lab even provided white boards and colored markers in places outside of the lab where chemists were likely to gather to talk informally over a cup of coffee or lunch. Pictures of structures and chemical

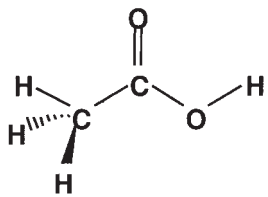

FIGURE 1 Structural diagram for acetic acid.

equations filled the glass panes of the hoods at each bench. Structural drawings were found in all texts related to chemistry work—in the notebooks kept by the chemists, on the labels for flasks and bottles, on posters in the hallways, even in the advertisements found in trade journals. Some of these ads contained very few words—just the name of the company and its address and the chemical name for the compounds sold—whereas the bulk of the ads were taken up by diagrams of chemical structures. The analysis of our observational data shows how chemists used these representations to do their work in the laboratory.

Data analysis. In the laboratories we observed, chemists used structural diagrams to give material reality to their thinking and to connect their thinking to the physical phenomena that was the focus of their work. An interview with James (represented as "J" in the protocols) illustrates how this was done.

James holds a doctorate degree and was at the time of the interview a senior chemist at the pharmaceutical company we studied. He had been an employee at the firm for the previous 10 years. James's group was responsible for synthesizing many of the compounds used by another group, the mass screening group, to ascertain which compounds are likely to be biologically active: a most important property for the chemicals that are synthesized in a pharmaceutical laboratory.

On the day we visited James's lab, he was working to create a compound that would be used as a reference for an assay. This was his third attempt to run this reaction; the previous attempts had failed. A flask containing the reactants was being heated in an oil bath and its contents were being stirred with a stirring bar. While the reaction ran, James took samples from the mixture to spot on a TLC plate. Other flasks contained the starting material and previously run reactions. He explained his work to Nancy, one of the coauthors.

J: There's actually a connection between these two things that are in the pot here and … maybe I can … wait while I get my pen.

What begins as a reference to a physical object on the lab bench—"the pot"—soon becomes a more extended discussion that is supported by a series of structural diagrams that James draws spontaneously (see Figure 2).

J: Okay. So, I'll draw these (1) out a bit. I'm just going to put some squiggly lines here (2) for the rest of the structure. The thing I'm trying to make looks like—looks like this (3).
   1 (Starts drawing the structures on the left or reactant side of the equation in Figure 2A.)
   2 (Completes the drawing of the first reactant.)
   3 (Draws out the first of the structures on right or product side of Figure 2A.)

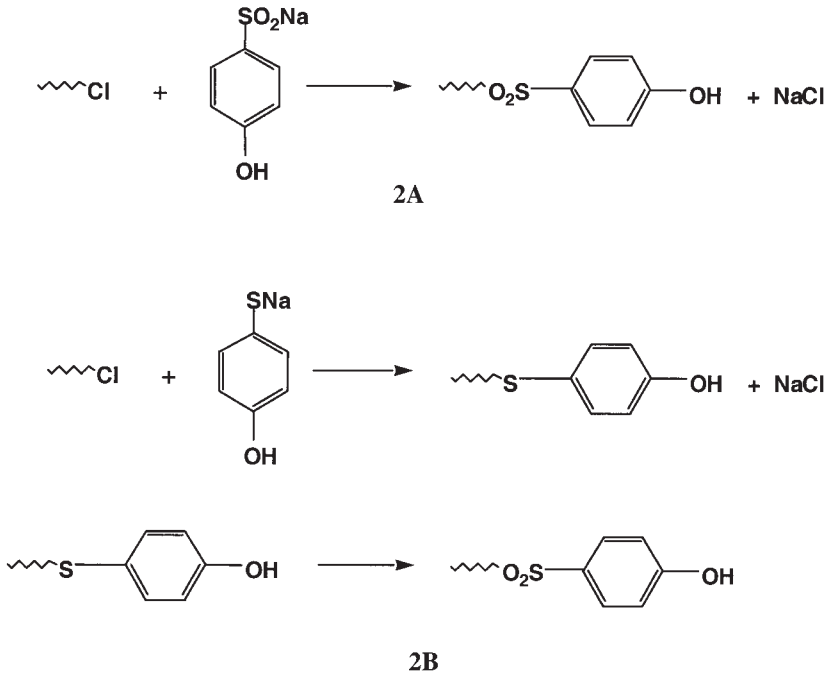

FIGURE 2 Approximation of James's drawing of the one-step (2A) and two-step (2B) reactions he was attempting.

There are four structures that James draws in Figure 2A that correspond to four substances. The two structures on the left side of the equation represent the starting materials (the "two things" in the pot). The separate physical existence of these two starting compounds has been perceptually obscured by the fact that they have been combined in the flask. Consequently, the first two diagrams in the equation serve to give these substances a separate material reality that can be referenced in James's explanation. The first of the two structures on the right side of the equation is the desired end product; the second is a byproduct. That these substances yet exist is neither perceptually apparent nor known at this point. These two structures in the equation serve a somewhat different purpose; they give material reality to what James would like there to be, the goal of his experiment. More specifically, the diagram shows what the target compounds should look like. However, in talking about how these substances should look, James is not referring to physical appearances but to how their atoms should be arranged in the compound. The features of the diagrams are in some way canonical to the presumed underlying structure. Thus, they allow James to "see" and reference the otherwise aperceptual objects of

this research and to see them in a particularly chemical way that is essential to the goals of his work.

The representations also help James think through and explain the process that is required to physically transform the starting materials into the target compounds and, correspondingly, to rearrange the atoms in the way he would like.

J: And so this is the nucleophile (1); this is the electrophile (2); and what you get out is sodium chloride.
1 (Points to the second structure on the reactant side.)
2 (Points to the first structure.)

This transformational process is both represented and supported by surface features of the diagram, features not otherwise available in the physical materials on the lab bench. James's reference to the nucleophile and the electrophile and the resulting sodium chloride that should come out of the reaction is an initial hypothesis of how this reaction should proceed. The representation allows him to "test out" his hypothesis by mapping elements of one structure onto those of another in a way that corresponds to the proposed mechanism of the reaction. However, James is also enacting the hypothesis and testing it with the physical materials of his experiment. Unfortunately, this particular experiment does not succeed.

J: But in my case that reaction is just not going. And so this thing (1) here that I'm filtering, I think it's yet another example of one of these that didn't go. I'm trying various things with the rest of this structure (2) to activate this ring and see if, see if I can get it to go, but I, I'm not very hopeful at this point.
1 (Points to the reaction flask.)
2 (Points to a graphic element in the second structure on the reactant side.)

Having made the connection between the diagrams and "this thing" in the flask, the physical consequence of "not going" has implications for the diagram. James's returns to the paper to develop a different mechanism that might alter the structure represented in the squiggly line drawing so that it would then enable the physical reaction to "go." He subsequently selects a different reagent and a two-step process to first produce a sulfur compound and then use an oxidation reaction to get the sulfur to a sulfoxide—the target product—along with the sodium chloride. In this way, his operations on features of the diagram have implications for his operations on the physical substances on the lab bench.

J: What I did was to take this reagent and we're going to do it in two steps (1). Take this guy (2) which is not the oxidized sulfur now but sodium sulfothiophenol which is a much better nucleophile. And so then I'm,

what I'm trying to do is to use this oxidation reaction (3) to get the sulfur to a sulfoxide. And so what, often times what you can't do in one step, you can do in two and it looks like that's (4) going to work.
1 (Draws a second set of reaction diagrams shown in Figure 2B.)
2 (Points to second structure on the reactant side of the first reaction.)
3 (Gestures toward the second step of the diagram.)
4 (Gestures toward a flask on the lab bench.)

This second, two-step procedure is supported by James's use of another diagram (see Figure 2B) to reason about other ways of "activating the ring."

The diagrams used by James represented both chemical concepts, such as "reactive sites" and "nucleophiles," as well as physical entities and processes, such as the substances in flasks and procedures performed on them. James moves back and forth between different surface features of the diagrams, such as nucleophiles and rings to work through ways of making the reaction go. However, because James was in the laboratory, he could also move back and forth between the diagram of possible problem solutions and their enactments in the flasks in front of him on the lab bench. Through this mediated, transformational process, he came to understand what was happening in the flasks and accomplished the goals of his work. This was a dual transformation: The materials in the flasks became "chemical" in a way that was not otherwise perceptible and surface features of the representations were used to transform the physical substances on the lab bench from a compound with one structure to another compound with a different structure.

The material nature of the situation James created allowed him to use gestures and make deictic references to both the features of the diagrams ("take *this* guy" and "*this* one") and the physical objects in the laboratory ("*here* in the other pot"). He created a semiotic equivalence: The "this guy" in the diagram is in some way the same thing as the "here" in the pot. Due to the situated nature of language use, he could then think about changes in the features of the diagram in ways that have implications for changes in the pot, changes that were not supported by the surface features of the pot—or language—alone.

The analysis of James's protocols makes it clear that there are certain features of structural diagrams that allow chemists to express both the current state of physical materials and the goals of their experiments in terms of the underlying structural composition and arrangement of atoms in the compounds. They can operate on these features in ways that allow them to reason through the actions that they perform on the physical materials in their laboratories.

Tool-Generated Representations of Underlying Structure

The representations that scientists generate to stand for the underlying structure of their desired products must be empirically verified against their associated phe-

nomena. Without this connection to the physical world, representations can become arcane and mystical, as they did with the prescientific phase of chemistry called alchemy (Crosland, 1962). Tools play an important role in making this connection. Although structural diagrams help chemists think about the aperceptual entities and processes that underlie their investigations, tools helped them test their thinking against physical phenomena they seek to influence.

A historical example draws on Lavoisier's own laboratory research. Tools played an important role in coming to understand the nature of gases—the research that led to a revolution in chemical thinking (Brock, 1992; Partington, 1989). The invisible character of most gases made it difficult for mid 18th-century chemists to understand them, as well as more visible, related chemical phenomena, such as combustion and acidity. The invention of tools such as the pneumatic trough, eudiometer, gasometer, combustion globe, and ice calorimeter—used along with the earlier technology of the balance—allowed 18th-century chemists to isolate gases and collect precise quantitative data about them. These new tools and their data allowed chemists to empirically "observe" otherwise invisible characteristics of gaseous substances, such as their mass. These data, combined with the new nomenclature, enabled Lavoisier to debunk the phlogiston theory and revolutionize chemical thought.

Similarly, the invention of new tools associated with the more recent shift from analysis to synthesis allow chemists to observe and verify their molecular structures. Although chemical synthesis became an increasingly common chemical activity in the late 19th and early 20th centuries, its progress at that point was impeded by the difficulty of confirming the structures of products that chemists intended to synthesize. It was not until new analytic tools became widely available in the 1960s that synthesis became a "contender for the heart of chemistry" (Hoffmann, 1995, p. 22). With these new tools, chemists could inspect structures and confirm in days findings that would have taken years to unravel in the 1940s (Brock, 1992).

In our observations in the academic and pharmaceutical laboratories, we encountered three types of instruments that chemists used most often: (a) TLC, (b) mass spectroscopy ("mass spec"), and (c) nuclear magnetic resonance spectroscopy (NMR). Like the technical tools of Vygotsky (1978), these tools mediate the work of chemists. However, they are unlike Vygotsky's technical tools in that they are not used to transform nature in a physical sense; rather, these analytic tools generate characteristic traces, such as streaks of color or peaks on a graph. Analytic tools, such as TLC and NMR, transform nature in a representational or semiotic sense; they generate a perceivable representation—a visualization—of some aspect of the chemical phenomenon that is of interest to the chemist and is not otherwise perceptually accessible. Obtaining these representations is not itself the desired goal of chemists; instead, they stand for chemical products that are desirable (e.g., the target compounds, their structures, etc.).

It is important to note that the representations generated by these tools are very different from those we observed chemists generating as an expression of their goals. The tracings of these tools look nothing like the structural diagrams that chemists use to communicate meaning to each other. Instead of letters and lines that stand for atoms, bonds, and their arrangements, there are streaks of color or peaks of various heights arrayed in various clusters and positions along an X–Y graph. Chemists use the features of these tool-generated representations to test, confirm, or refute the composition and structure of the compounds they synthesize.

Due to the fact that there are many potential compounds that could result from reactions of a given set of reagents and many permutations of their atomic arrangements, there are a large number and variety of patterns that chemists can encounter with tool-generated representations. The meaning of all but the most common spectra is open to question and negotiated between the chemists. These negotiations depend heavily on social discourse in the context of representations and their features. In this section, we concentrate on how the surface features of the tracings generated by these representational tools are used by chemists to verify or refute the results of their investigations. In the subsequent section, we focus on the social discourse that is the basis for the interpretive process.

Before proceeding to a description of how chemists interpret these representations, we provide a brief introduction to one of these instruments, an NMR. For some readers, it may be sufficient to say that the NMR generates a graph called a spectrum. The shape and position of peaks on the spectrum are characteristic of specific structural components of the molecule. The interpretive task of the chemist is to analyze these patterns and infer the composition and structure of the entire molecule. Readers who are satisfied with this description can move directly to the data to get a general sense of the interpretive process. Readers interested in a more detailed analysis of the protocol would benefit from reading the Appendix, although this will require some understanding of basic chemistry.

Data analysis. An interaction with Susan, a senior synthetic chemist at the pharmaceutical lab, illustrates how chemists use the features of NMR spectra to examine the products of their research. Susan (represented as "S") holds a doctorate in chemistry and has been employed at the pharmaceutical firm for several years. At the time of this study, she was working with a group on developing drugs for neurodegenerative diseases, like Alzheimer's. This conversation took place in Susan's office.

During the conversation, Susan worked on three different NMR spectra for reactions she had run in her laboratory earlier. We have displayed a spectrum for a compound similar to that for one of the reactions (see Figure 3) and a structural diagram of that compound (see Figure 4). Susan did not draw a diagram of the com-

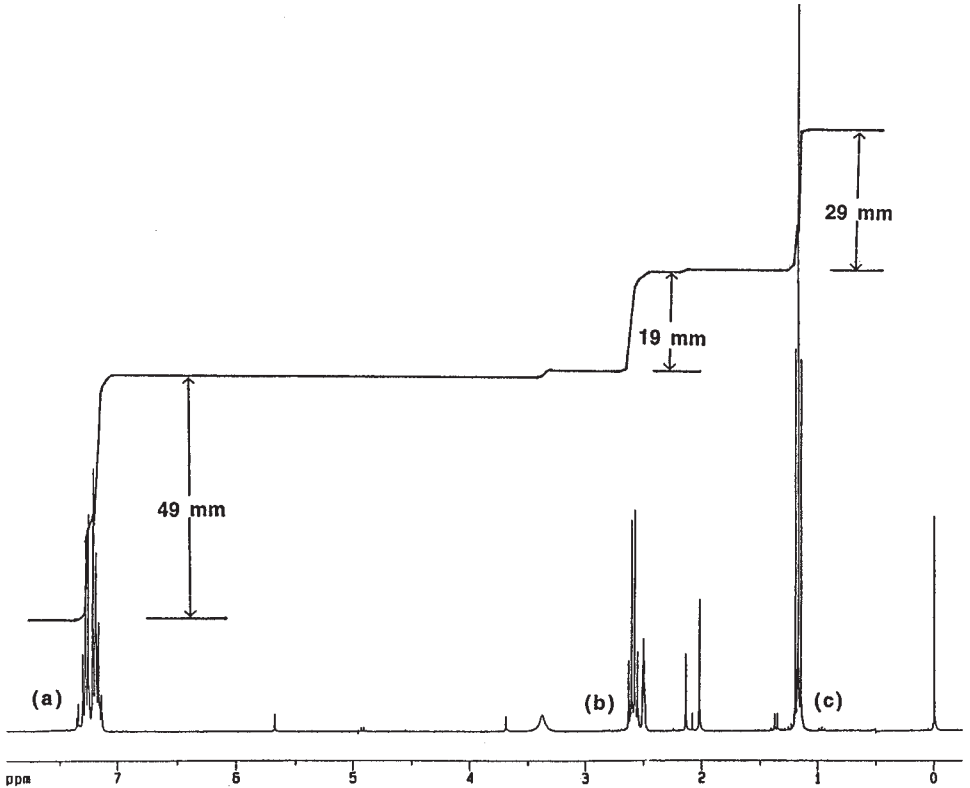

FIGURE 3 Approximate NMR spectrum for reaction described in Susan's protocol. The letters *a*, *b*, and *c* are for reader's reference and do not appear on the NMR spectrum.

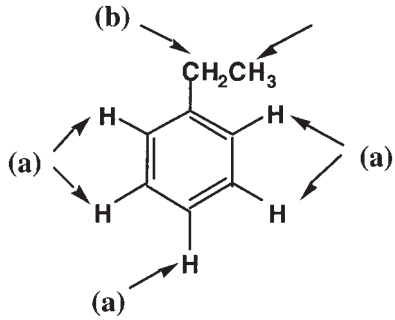

FIGURE 4 Structural drawings for the compound that generated the spectrum in Figure 3. The lowercase letters (a–c) correspond to the labeled peaks in the spectrum.

pound but we include one for the reader's reference. Due to our agreements with the pharmaceutical company regarding the confidential nature of their intellectual property, we have selected a spectrum for ethylbenzene, a simpler compound but one containing some of the components of the one Susan synthesized. We have made minor changes in the protocol to protect confidentiality and maintain a correspondence between the protocol and the ethylbenzene spectrum.

During this session, Susan uses the NMR spectra to make two interrelated decisions about her lab work:

1. Does she have an acceptable spectrum?
2. Did she synthesize the intended compound in her laboratory work?

She begins the session by pulling a book down from a shelf.

S: Now I'm just going to look up … now this is the book that Joe was talking about, that, there's one section that's just on NMR. It talks about the theory but it also has some very practical things about where shifts would be.

By drawing on a reference book, Susan connects her interpretive work to that of a larger community of chemists, both her colleague (Joe) who suggested the book and the chemists who produced the spectra included in its pages. She begins moving back and forth between a spectrum in the book and one in front of her to see if she synthesized the product she intended.

S: This, this triplet (1) should be this (2), these three protons right here and this (3) looks like one of these (4), and this (5) looks like one of these (6). And the reason I say that is that they're just a bit broader.

These are a quadruplet (7), which is the split that you would expect from those. And then the rest of these are aromatics (8). So you have, one, two, three, four, five, six, seven, eight (9). You can almost count these. One, two, three, four, five six, seven, eight (9). And then this one (10) is one of the other ones. So, it looks about … and that looks really nice.

1 (Points to Cluster C the spectrum in Figure 3 [labels do not actually appear on the spectrum].)
2 (Points to a peak on a spectrum in the book.)
3 (Reference to the spectrum.)
4 (Reference to the book.)
5 (Reference to the spectrum.)
6 (Reference to the book.)
7 (Points to Cluster B on the spectrum.)
8 (Points to Cluster A on the spectrum.)
9 (Counts peak in Cluster A.)
10 (Reference to spectrum.)

The clear delineation of features of the spectrum conforms to expected patterns and this leads Susan to feel comfortable that it is a "nice looking" spectrum that she can use in her analysis. As she works through different features of the spectrum, noting the triplet, three types of protons, and the quadruplet, each of these patterns contributes to an emerging interpretation of what Susan hypothesized should be present in the compound. At the same time, the emerging interpretation of the composition of the compound contributes to her confidence in the quality of the spectrum. The pattern for the aromatics and the way their peaks can be easily counted clinches the assessment: "and that looks really nice." Earlier she had rejected two other spectra, based on their features, because one was "not phased right" and the other was "just not a very good spectrum." By confirming the validity of the spectrum in Figure 3, Susan has made a semiotic connection between it and the substance on her lab bench.

Having made the connection between the spectrum and the physical material that she synthesized, Susan must determine the composition, structure, and consequently, the identity of the material she made. She returns to the spectrum and works through a more refined interpretation of what is present there, an analysis that will allow her to determine if she has synthesized the product that she wanted.

S: So measure these, and see (1), so that's about 180, and this is methylene chloride, I'm pretty sure. Right shift that. This is 30, 75, 77 (2). So that means, it's not, so that means, I know I have five protons here in the aromatic region. One-eighty divided by 5 equals (3) …, so each proton should be about 36. So that should be five protons. This is, I

should integrate for about 83. So that could be one you know you dumped. That's about 2.1, round to 2. Seventy-seven (4), so I've got more protons on the molecules than I should have.
1 (Measures integration curve above Cluster A with a ruler.)
2 (Measures other parts of the integration curve.)
3 (Performs division.)
4 (Uses calculator.)

Susan takes out a ruler and measures the various peaks appearing on the graph. She uses a calculator to figure the integration step heights of the total peaks in the aromatic ring: 180. She measures the other integration lines, as well. Due to the fact that she knows there are five protons in the aromatic ring, she divides 180 by 5 to get 36, the relative value for a proton in this spectrum. She then can divide the other integration measurements by 36 to determine the number of protons in each set of peaks corresponding to segments of the molecule and sum these to determine the number of protons in the entire molecule. These calculations lead her to the conclusion that "I've got more protons on the molecules than I should have." That is, although she used the peaks to determine that she has an acceptable spectrum, additional analyses of these peaks tell her she does not have the compound for which she had hoped.

Again, notice the specific features of the representation in Figure 3 that Susan must work with. The lines and peaks arrayed along the axes of the spectrum look nothing at all like the structure of the compound that generated it, at least as this structure is represented in the diagram in Figure 4. The molecular components are not there for Susan to see, as they are in a diagram. She must literally construct an understanding of the spectrum by operating on its features and transforming them from peaks to chemical entities. The peaks in the spectrum (Peaks A, B, and C) are mapped onto similar features in the references book and ultimately to features on the structure of the molecule (as they correspond to Figure 4). By measuring the peaks and performing mathematical calculations on them, she transforms one type of representation of the phenomenon (the peaks generated by the NMR) into another type (the number of protons in the structure). By coordinating these resources in this manner, the substance Susan synthesized in her lab comes to be a molecule of known composition and arrangement, although not the one she had hoped for.

The analysis of Susan's protocol shows how chemists use tool-generated representations to confirm or refute the results of their investigations. This is a two-step process whereby scientists first confirm a valid connection between the representation and the phenomena that they study and then they interpret the meaning of the representation. This is a social, rhetorical process in which specific features of representations serve as warrants to claims, as demonstrated in the following section.

Social Discourse and the Confirmation of Underlying Structure

In our observations so far, we saw how James used diagrams to represent the structures of the physical substances he was working with in his laboratory, and we saw how Susan used NMR spectra to empirically specify the structure of the material she had synthesized in her laboratory. Due to the fact that James and Susan were working alone in their laboratories and offices, the fundamentally social nature of their work was not apparent. Yet in their individual work, James and Susan recapitulated social, rhetorical processes that we observed in more overtly social contexts as chemists worked together. For example, when Susan accepted the spectra but found she had more protons than she wanted, she was reflecting the rhetorical interactions we observed between chemists as they discussed and argued about the products of their work: interactions of the sort that we examine in the following protocol between David and Tom.

By examining a pair of chemists as they use representations in the laboratory, the social nature of this process becomes explicit. We see how an understanding of the aperceptual, underlying structure of substance is a coconstruction that depends on the ability of chemists to coordinate features within and across different representations to build a compelling argument that supports a proposed structure. We also see how representation use both draws on and contributes to accumulated information and evidentiary conventions within a community of practice to which chemists belong. Finally, we see how the use of representations supports the "coming to participate" of a new member of the community. The following protocol shows that one moves from peripheral participation in a community to full participation in part by using its tools and representations in the context of activity and discourse (Lave & Wenger, 1991).

We conclude the article with a discussion of educational implications of this detailed look at the discourse and representation use of scientists. We explore how the use of representations within discourse may contribute to the development of a community of learners in chemistry. We look at how technology-augmented environments can be designed to provide students with representational tools that can support their chemistry investigation and talk, increase their chemistry understanding, and assist their coming to participate in a chemistry knowledge-building community.

Data analysis. The following example is drawn from our observations of chemists in the academic laboratory. In this example, Tom, a 2nd-year doctoral student in chemistry discusses the progress of his bench work with his faculty advisor, David. Before entering graduate school, Tom had spent part of his senior year in college working in a research laboratory at another university. In addition, he had

spent a summer working for an industrial laboratory. At the time we observed this interaction, Tom had worked for David's research group for about 1 1/2 years.

The discussion began with David asking Tom to describe his results from the latest series of reactions he has run. David and Tom left Tom's bench and walked over to a whiteboard located at one end of the lab. Tom first drew the chemical structure of the starting material on the whiteboard (see Figure 5) and the reagent (Lawesson's). He then drew another structure of an intermediate compound and an arrow with the chemical formula Me_2SO_4 written above it.

This is a two-step synthesis (leading to yet other reactions) in which Tom wanted to attach a methyl group (CH_3) to the sulfur (S), as depicted in Figure 6. However, the end product depicted in this figure was not drawn. Instead, Tom referred to it as "some compound." This does not mean that Tom did not have a particular compound in mind as the goal of his synthesis; rather, it acknowledges the fact that he did not know if the material on the lab bench was the target compound. His task at this point was to explicate the structure of this product to see if he had the intended compound. He was careful to tell David the amount of starting material used in the reaction (1 1/2 grams) and the yield from the first reaction—49%—and this was also drawn on the whiteboard. The following excerpt takes place back at Tom's desk as he shows David the C–13 (carbon 13) and H–1 (proton) NMR spectra that were run on this compound.

The representations that are of primary focus in their discussions are the NMR spectra. As with Susan's protocol, the meaning of these spectra are not at all transparent—even to David, the professor.

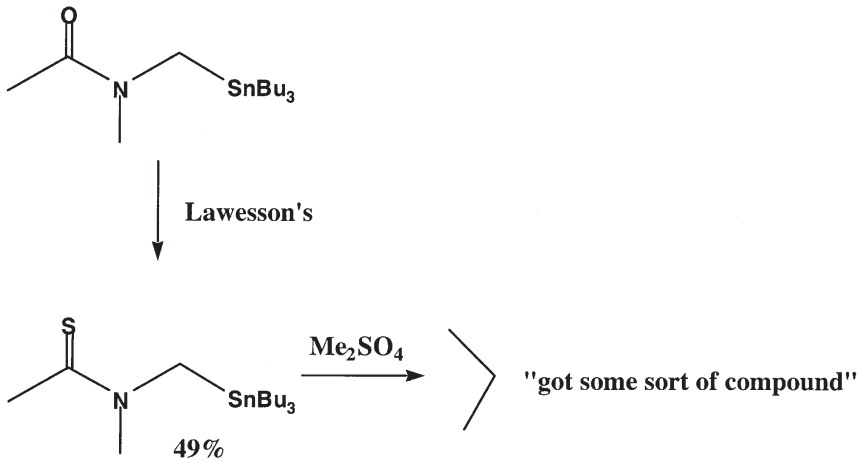

FIGURE 5 Tom's drawing of the reaction.

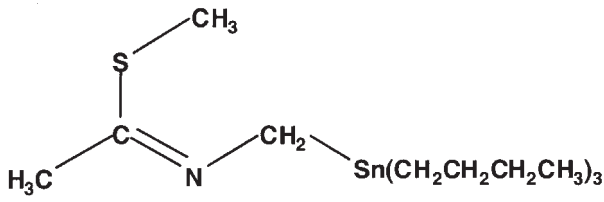

FIGURE 6 Structure of the compound that Tom and David were trying to synthesize.

D: Well, weird, uh, let's take a look at it. I mean, is it mostly one compound or a bunch of compounds?
T: I don't even know that. Um, I don't have enough data on that stuff.

It is relatively easy to identify some of the constituent atoms and David uses features of the NMR spectrum to do so.

D: Oh, my gosh, there are clearly some minor compounds in here. … Well, it's got tin in it (1).
T: Oh, yeah, it's definitely got tin in it.
D: It's got a couple of methyl groups (2); that's good.
1 (Points to peaks on the NMR that indicate the presence of tin.)
2 (Points to two other peaks that correspond to the methyl groups.)

However, the rest of the spectrum is more problematic. David begins to propose possible alternative structural arrangements, specifically the possibility that they have a mixture of two geometric isomers where the S-CH_3 and the CH_3 groups off of the carbon (see Figure 6) are transposed. They refer to these as the E and Z isomers.

D: Well, could we have an E and Z mixture?
T: Oh, I don't know.
D: OK, you're expecting it to look like a singlet with two tin satellites, right?
T: That's right, yeah. And if it's E and Z, I think it would effect these (1) somewhat.
D: OK, wait, now let's see. So we would expect to see, OK, we see two methyl groups.
1 (Points to a set of peaks.)

By rejecting David's proposed mixture, Tom begins to take a role in the discourse. However, he does not reject David's comments out of hand. It is important

to note that Tom begins by accepting David's point about the expected single peak. Tom then goes on to use additional features of the spectrum as evidence that contradicts other expectations implied by David's proposal.

As the discourse progresses, it becomes a complementary, dialogical process between two interlocutors. Sometimes David asks a question and Tom provides an interpretation; sometimes Tom asks a question and David provides an interpretation. Sometimes Tom makes an assertion and David questions the evidence; sometimes it is the other way around. Although the process is complementary, it is not symmetrical. During the period of our observation, David does most of the questioning, asking 17 questions to Tom's 4. He also offers several possible structures and guides much of the interpretation of the spectra. Apropos his status as a graduate student, Tom has not yet come to fully participate in this process. Yet there is a significant segment of the protocol in which Tom shows that he is moving toward full participation, however tentative that movement is.

D: What are these two peaks down here?
T: Um, those are tin satellites. Um …
D: Um, why would they be on one methyl, oh, the other one's off the sulfur.
T: The, the, the, actually the sulfur, when I do the O-methyl case, that O-methyl group, shows tin satellites.
D: No.
T: Yes, yes.
D: And the C-methyl doesn't?
T: The C-methyl does not.
D: How do you know this, how do you know the assignment?
T: Uh, uh, I'm assuming by shift.

When David considers the interpretation of two peaks, Tom asserts that they are influenced by the tin and goes on to contend that the peaks are associated with the sulfur-methyl. Tom cites the results in a similar experiment as supporting his assertion ("the O-methyl case"). This was a previous experiment of Tom's and David does not have direct access to information from it. This information that Tom has that David does not allows Tom to take a stronger rhetorical position in the interpretation. This role is tentative, at first. However, later in the protocol, Tom goes on to develop his analysis and begins to move David toward his position.

As David works through the implications of Tom's argument, he spontaneously generates a diagram of the proposed structure and uses this to test the proposed interpretation against the spectrum.

D: Let's see, so that would be uh, this compound here. So I got to write it out to think about it (1). … OK. Well, uh, you got to keep the C-13 here. Uh, is this where you expect the amine to be (2)?

T: Yes.
D: Where would the thiocarbonyl be?
T: Uh, I'll find out (3).
1 (Draws a diagram of the proposed structure.)
2 (Points to a portion of the carbon-13 spectrum.)
3 (Pulls a reference book from a shelf.)

David and Tom are now coordinating the features within and across the C-13 and H-1 NMR spectra, a diagram, and a reference book. In using a diagram, David is making the proposed structure explicit in a way that allows him to test it against the spectra. In using the tool-generated spectra, they are connecting this interpretation of the structure to data from their experiments. In using the reference book, Tom is connecting their interpretation to the previous experiments of others in the chemistry community. Nonetheless, the confirmation of the interpretation rests on the argument that David and Tom are able to construct using the resources they have assembled. By this point in the analysis, Tom has come to build a compelling case. David confirms this, again by referring to features of the representations.

T: I don't know. I mean, I would be skeptical but the proton is, uh … I mean clearly there's the NH (1).
D: NH.
T: I mean it's, it integrates beautifully.
D: Oh, OK, so that's the C-methyl (2).
T: Uh hum.
…
D: So, 2.25 is probably good. Look at that (3), right where you would expect. S-methyl?
T: C-methyl. You don't have a …
D: That's good. Well, like you said there seems to be another. … I don't think, I think it could be easy. If you say, so, let me get this straight, if this is two (4), then the total of these three peaks would be six.
T: Yes.
D: Sounds good to me. That's a very attractive explanation there.
1 (Refers to peaks on the NMR.)
2 (Refers to peaks.)
3 (Refers to an area of the NMR.)
4 (Refers to an area of the NMR.)

Even though David is a professor and Tom is a graduate student, this conversation was similar to others we observed between professional chemists. It differed more in its lack of symmetry than in its structure. During the session we observed, 19 references were made to the spectra and their features; 13 of these were made by

David and 6 were made by Tom. Even though Tom made fewer references to representations than did David, his use of the representations were very similar to his professor's. In his talk, Tom used specific features of representations as evidence to argue for the underlying structure of the products that were synthesized. Based on this evidence, both Tom and David come to believe that the aperceptual molecules of their reactions are arranged in certain ways.

Tom's use of representations serves two important functions. First, in interpreting spectra, Tom learned chemistry. He did not just learn new knowledge about the structure of specific molecules and how they can be synthesized, rearranged, and analyzed. Tom was also learning how to "talk chemistry"—How to take a position, create an argument, and use representations to support his position. Second, interpreting representations was the principal activity in which Tom and David were engaged. This was not an artificial activity that David has contrived for Tom's edification but one that is central not only to the function of David's academic laboratory but to chemistry in the outside world, such as that practiced in James' and Susan's pharmaceutical laboratories. In using and interpreting NMR spectra and other representations on this occasion and others during his graduate work, Tom was engaged in a primary activity of the chemistry community and as a result was becoming a member of that community.

The social nature of representation use among chemists is demonstrated by the analysis of Tom's and David's protocol. Specific features are used as rhetorical devices to warrant claims about the findings of scientific investigations. Furthermore, the use of representations and tools in this way confirms membership in a community of scientific practice.

REPRESENTATIONS AND TOOLS FOR KNOWLEDGE-BUILDING COMMUNITIES

As mentioned at the start of the article, several educational researchers (Brown & Campione, 1994; Scardamalia & Bereiter, 1994a) have used practices of the scientific community as a metaphor for the design of educational activities and environments. For example, Scardamalia and Bereiter (1994a) referenced the practice of scientists when they define knowledge-building communities as people engaged in producing knowledge products that lend themselves to being discussed and tested. These knowledge products (e.g., publications and oral reports) constitute some advance over what is already known, as locally determined. The researchers go on to describe communities of students that are similarly focused on the shared task of building knowledge rather than the individual task of memorizing established fact. Like scientists, students in these knowledge communities engage in discourse and generate reports focused on scientific phenomena. In doing so, they identify problems that need to be solved or explained, ask insightful and critical questions, and

advance theories and use these to explain results. In explaining results, students describe how things work, propose underlying causes and principles, and explicate the interrelatedness of ideas. Scientific modes of thinking, such as conjecture, speculation, evidence, and proof become part of the common voice of the community (Brown & Campione, 1994). Discussion, questioning, and criticism are the mode rather than the exception.

Roth and McGinn (1998) suggested that the use of representations should be central to the practices of these knowledge-building communities as a way to both support student understanding of symbolic inscriptions and develop their understanding of the scientific phenomena that these symbolic expressions represent. This position is supported by our historical and observational study. The findings of this study provide some of the details of scientific representational practices that can inform the use of representations within student communities. The question addressed in this article is, How does an understanding of the representational practices of chemists in their laboratories contribute to the knowledge building practices of chemistry teachers and students in classrooms?

We explore these implications in the context of a new project, called *ChemSense* (Coleman, Kozma, Schank, & Coppola, 1998), which extends our earlier work (Kozma, in press; Kozma & Russell, 1997; Kozma, Russell, Jones, Marx, & Davis, 1996; Russell et al., 1997) and a project-based inquiry approach to science learning (Krajcik et al., 1998). A significant national goal for science education is to engage students in direct experience with the methods and processes of scientific inquiry (Advisory Committee to the Education and Human Resources Directorate of the National Science Foundation, 1996; American Association for the Advancement of Science, 1993; National Research Council, 1996). This curricular orientation links student classroom activities to the laboratory practices of scientists in a more direct way than previous curricular orientations. Findings in the Krajcik (1998) study and others (Metz, 1998; Roth & Roychoudhury, 1993) demonstrated that even young students (i.e., middle school) can fruitfully engage in scientific investigation. With Krajcik's approach, students conduct extended projects in which they pose scientific questions, plan and design investigations and procedures, construct apparatus, carry out their experiments, interpret data, draw conclusions, and present their findings. Although not explicitly connected to the knowledge-building framework, Krajcik's approach to science learning is quite compatible with it because investigations are collaborative and because the approach engages students in knowledge-building discourse activities, such as questioning, explaining, presenting findings, and so forth.

The findings of our study of scientists' use of representations argue for the use of similar representational practices by science students as they engage in investigations and build knowledge in science classrooms. There are two interrelated components to these recommendations: the development of representational skills

as part of the chemistry curriculum and the use of these skills to better understand the chemistry that underlies student investigations.

Our findings in this study and our earlier laboratory research (Kozma & Russell, 1997) document that chemists have a set of representational skills or competencies that are central to their understanding of chemistry and the conduct of their work. These skills allow them to move flexibly between different types of representations and use them together to express their ideas and to understand their domain. Such findings from the studies of experts have often been used to identify curricular goals for students, that the knowledge and skills of experts are appropriate models for student knowledge and skills (Glaser, 1989, 1990). Based on the findings from these studies, we recommend a set of representational competencies that should be part of the science curriculum. Science courses should strive to develop students' ability to

- Generate representations that express their understanding of underlying entities and processes.
- Use these representations to explain chemical phenomena at the observable, physical level in terms of chemistry at the particulate (i.e., molecular and structural) level.
- Identify and analyze features of a representation (such as a peak on a graph) and use them to explain, draw inferences, and make predictions about chemical phenomena or concepts.
- Take the epistemological position that representations correspond to but are distinct from the phenomena they observe and their understanding of it.
- Use different representations that are appropriate for different purposes.
- Use language in a social context to communicate chemical understanding and make explicit connections across representations that convey relationships between different representations and between symbolic expressions and the phenomena they represent.

Whereas studies of expertise provide us with insight into the skills and knowledge of scientists, which can serve as models for student knowledge, observational studies provide us with an understanding of the ways scientists use their skills and knowledge in the context of their investigations as they come to know. These observational studies provide us with models of how students may use these skills within the material and social contexts of their classroom investigations and knowledge building communities. From this perspective, the curricular goals related to representational competence are both accomplished by and in turn contribute to the use of representations by students engaged in project-based inquiry. The findings of this study suggest a number of ways that teachers and students may use representations as they pose questions, plan investigations, construct apparatus, carry out their experiments, interpret data, draw conclusions, and present their findings.

For example, the findings suggest that teachers should engage students in the use of representations to pose the research questions, make predictions, or state the goals of their investigations. As they did for James, the features of representations (e.g., molecular diagrams) can help students describe their investigations in terms of the processes that they would like to occur and the chemical entities they expect will result from their experiments. When designing their investigations, students should be prompted to think about the representational form of the data they will collect, how it will be displayed, and why a particular display might work better for their purposes than another. When constructing their apparatus, they should describe the relation between the physical changes they expect to observe and the data that are generated by instruments. Increasingly inexpensive sensors and probeware (e.g., pH meters, temperature probes, conductivity meters, etc.) can connect representations to physical phenomena, as the NMR did for Susan. The representations generated by these instruments can support students' discussion of physical changes in terms of the features built into these displays (e.g., axes labeled pH and concentration), features that correspond to both physical observations and underlying chemistry. As did Susan, students should interpret their data by using specific features of the data display to think about and explain the perceptual phenomena of their observations in terms of aperceptual entities and processes. In presenting their findings, students should use these displays along with other representations to explain their findings and argue for their conclusions, as did David and Tom. In this regard, it is particularly important to use the features of several representations together (particularly student-generated and empirically generated representations) to explain the results, as the correspondence between features (or lack thereof) can serve as the warrants for confirming or disconfirming conclusions about findings. By using representations in these ways, they become part of the discourse and meaning making of the knowledge-building community. These practices in turn develop the representational competence of students and the use of representations by students to understand chemistry.

However, it is also important to acknowledge that there are significant differences between scientists and students and these differences must qualify the implications we derive from our results. For example, high-school students or even undergraduates are not likely to conduct chemical synthesis, the core activity of all the chemists we observed. Nonetheless, students need to understand the underlying chemical entities and processes that underlie their simpler investigations (American Association for the Advancement of Science, 1993). The ability of James to quickly sketch the molecules involved in his experiments and his ability to make connections between nucleophiles and electrophiles denotes a significant amount of current knowledge about entities and processes that support his use of representations. It can not be assumed that students have this understanding (Krajcik, 1991; Nakhleh, 1992). Susan's ability to transform one symbol system into another helped her interpret the meaning of her spectra. Even college chemis-

try students are not proficient at transforming representations (Kozma & Russell, 1997). Both David and Tom drew on evidentiary conventions of the chemistry community to make their case for an interpretation of the spectra. Students rarely produce explanations or justifications for their positions (Coleman, 1995; Coleman, Brown, & Rivkin, 1997). These differences also have implications for representational practices and resources in the classroom.

Our historical analysis makes it clear that the way representations are designed both shapes and is shaped by the activities of the scientific community and their understanding of scientific phenomena. Consequently, the representation resources and representational practices that are used in the classroom need to be specifically designed to support the goals and needs of the nascent knowledge-building communities of students. Given the practices of scientists and the needs of students, we have derived some specifications for the design of representational environments to support the investigations of these knowledge-building communities. The details by which these specifications would be implemented are currently being developed in our *ChemSense* project (Coleman et al., 1998).

We propose these specifications in the context of representation-enriched technological environments. Computers can be distinguished from other media by their advanced symbolic and processing capabilities (Kozma, 1991). These capabilities are beginning to be used by the educational research community to develop advanced representational environments in science (Dede, Salzman, Loftin, & Ash, in press; Edelson & Gordin, 1998; Horwitz & Christie, in press; Jackson, Krajcik, & Soloway, in press; Rochelle, Kaput, & Stroup, in press; White & Frederiksen, in press). Such technological environments can provide students with the material and social resources that can support their investigations, discourse, and knowledge building. Based on the findings of this study, we recommend that these environments should be designed with certain features and capabilities that provide students with

- Specialized symbol systems and tools that allow students to express their understanding of invisible chemical entities and processes. These could include specialized graphics packages, such as molecular drawing and modeling packages that are similar to those used by scientists. However, they may also include animation tools that allow students to explicitly illustrate these processes. Chemists do not have tools like this; processes are often implied or denoted with a simple arrow or squiggle. However, the features of these symbol systems that correspond to entities and processes that are otherwise unfamiliar to students gives them new ways to think and talk about science that goes beyond the surface features of the physical phenomena (Kozma, 1999; Kozma et al., 1996).
- Tools and scientific instruments that students can use to empirically generate real-time representations of physical phenomena and connect these representations to those that students generate. Real-time representations can support student

discourse as they try to understand the physical phenomena that generate them (Kelly & Crawford, 1996). By creating tools and tasks that require students to annotate and explain the features of these tool-generated representations, these technology-based environments can help students explain the features of one representation using those of another. Alternatively, the system could support these cross-representation transformations by providing tools that automatically highlight the feature of one representation (e.g., number in a spreadsheet) when a feature of another (e.g., a peak on a graph) is selected.

- A multirepresentational communal database that structures and scaffolds students' learning conversations. The database should allow students to generate notes with their ideas, explanations, predictions, and questions about the phenomena they are investigating. The system should allow students to connect these notes to features of representations that they generate and those that are generated by probeware and data. They could also be connected to features across representations in a way that supports student discussion of the relation of one representation to another and to underlying chemistry.

The teacher must play a key role in the use of such environments; they do not stand on their own. The kind of discourse and representation use that is desired of students would need to be modeled by teachers, much as David modeled the process for Tom during their collaboration. As they discuss investigations with students, teachers must demonstrate how to use representations to ask questions, interpret findings, and draw conclusions. As a consequence, the community of students will be able to collaborate on the creation of an extended body of knowledge related to their investigations that has representations and representational use at its core.

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APPENDIX

NMR Spectroscopy

Two types of NMR spectra were used by the chemists we observed: proton NMR and carbon–13 NMR. An NMR is used to identify the arrangement of specific types

of atoms in a compound. The proton NMR is used to analyze the arrangement of hydrogen atoms and the carbon–13 NMR is used to analyze carbon atoms. Both of these are of particular importance to an organic chemist. The identification of the arrangement of these atoms aids in the confirmation of both the composition and structure of the entire compound.

With either NMR, the analysis starts by dissolving a sample in a solvent that does not influence the NMR spectra. Once placed in the NMR spectrometer, the sample is subjected to both a strong magnetic field and radio frequency (RF) radiation. When molecules are exposed to the magnetic field, about half of the nuclei align with the field; the other half—those with more energy—align against the field. RF energy is applied to the sample to bring the nuclei at the lower energy state to the higher energy state and thus to flip their spin alignment against the magnetic field. The exact amount of energy (frequency) needed to do this depends on the strength of the local magnetic field as it is experienced by each proton. The strength of the magnetic field experienced by each proton is modified in characteristic ways by the other protons and electrons in its immediate vicinity; in a sense, they shield the proton from the applied field. The greater the electron density around a proton, the more RF energy will be needed to induce it to align opposite the magnetic field. Thus, the amount of energy absorbed is an indication of the molecule's structure.

The NMR generates a spectrum that plots absorption intensity on the *y* axis versus chemical shift (or δ) on the *x* axis (see Figure 4 for a sample spectrum). Chemical shifts are characteristic of the types of proton arrangements found in molecular units. For example, methyl (CH_3) is a structural component commonly found in organic compounds. The three protons (H) of the methyl group show a chemical shift (in the 0–2 δ range). The sift for the protons on a benzene (or "aromatic") ring would appear in the 7 to 8 δ range. Thus, the chemical shifts of peaks observed in a NMR spectrum provide evidence for the existence of specific types of molecular and submolecular structures.

Chemists also use information contained within the peaks themselves. Some peaks will appear not as a single peak but as a cluster of equal-strength doublets, triplets with a 1:2:1 intensity ratio, or quartets with a 1:3:3:1 ratio, and other specific patterns that depend on the number of equivalent protons bonded to adjacent atoms. Superimposed on the peaks is a second graph, an integration graph, that displays the cumulative areas under each peak. This provides chemists with information on the number of protons of each type in the sample.

In interpreting NMR spectra, chemists analyze the patterns of the positions, number, and relative sizes and areas of the peaks to identify compounds and their structures. A spectrum can be compared with those in a reference book to identify a common compound, or chemists can use features of the NMR spectrum to construct an understanding of the identity and structure of the compound, component by component. The latter is likely to be necessary for the synthesis of a novel compound.