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Paper 2

The Role of Representations in Problem Solving in Chemistry

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Abstract

For ten years, we have been studying the differences between successful and unsuccessful problem solvers. It doesn't seem to matter whether the study examines students' ability to solve multiple-choice stoichiometry questions during a general chemistry course, students' ability to solve complex synthesis questions in an advanced-level course on organic synthesis, or any course between these extremes. In each case, students who use symbolic representations are more likely to be successful than those who don't, and students who construct more than one representation during their search for the solution to the problem are more likely to be successful than those who don't.

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INTRODUCTION

Several years ago, students in the first-semester of an organic chemistry course for nonmajors were given an exam on which the question in Figure 1 appeared.

Provide the systematic (IUPAC-approved) names for these compounds

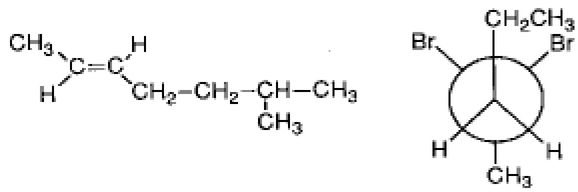

Figure 1.

Most of the students successfully named the compound on the left, but not the one on the right. The students weren't much more successful at naming the compound shown on the right when this part of the question was repeated on the next exam. Or when the same question appeared on the final exam. The students' success (or lack thereof) on this question isn't as interesting, however, as their response to the question when they were interviewed. Time and time again, we heard students comment that the question wasn't "fair."

A similar phenomenon was observed when the following question appeared on an hour exam for the second-semester course.

> A graduate student once tried to run the following reaction to prepare a Grignard reagent. Explain what he did wrong, why the yield of the desired product was zero, and predict the product he obtained.

$$CH_3CH_2Br \xrightarrow[CH_3CH_2OH]{Mg} CH_3CH_2MgBr$$

When he wrote the exam, the instructor (GMB) was convinced that this was a relatively easy question. (There is nothing wrong with the starting material, which is a common reagent used to prepare Grignard reagents. There is nothing wrong with the product of the reaction, which is a typical Grignard reagent, or with using magnesium metal to prepare this reagent. The only possible source of error was the solvent: CH_3CH_2OH.) He therefore used this item as the first question on the exam - to build the students' confidence.

When the exam was graded, he found that some of the students recognized that the solvent was a source of H^+ ions that would destroy the Grignard reagent produced in this reaction. But many of them were unable to answer the question, and, when these students were interviewed after the exam, they frequently expressed the opinion that this wasn't a "fair" question.

The primary goal of this paper is to develop a theoretical explanation of the difference between the students who were successful on these questions and those who were not. A subsidiary goal, as you might expect, is to explain the source of students' beliefs that these questions weren't "fair." Before we do this, however, it might be useful to analyze student responses to one more exam question, based on the reaction shown in Figure 2.

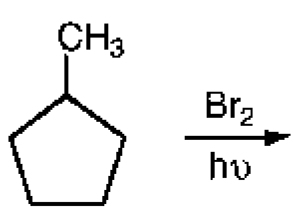

Figure 2.

The students were asked to predict the major products of this reaction, estimate the ratio of these products that would be formed if Br� radicals are just as likely to attack one hydrogen atom as another, and use the relative stability of alkyl radicals to predict which product is likely to occur more often than expected from simple statistics.

Most of the more than 200 students in this course predicted that the reaction would give the three products shown in Figure 3, with a relative abundance of 3:2:2.

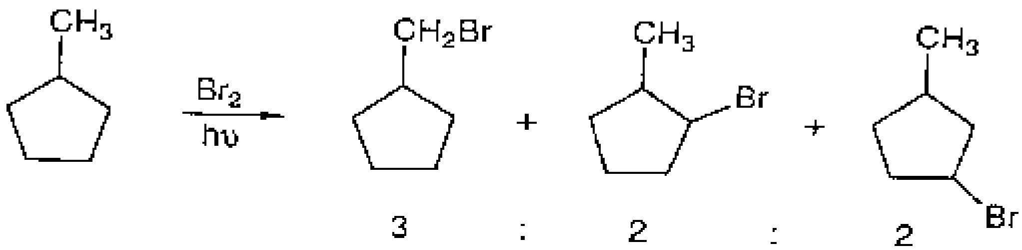

Figure 3. The most common answer.

When we discussed their answer with these students we found that they recognized that attack by the Br� radical at any of the three hydrogen atoms in the CH_3 group would give the first product. They also recognized that the molecule is symmetrical, and it therefore doesn't matter whether reaction occurs on the right or left side of the molecule when the second and third products are formed. Unfortunately, they failed to recognize that there are *two* hydrogen atoms on each of the carbon atoms at which attack occurs to give the second and third products. They therefore failed to recognize that simple statistics predicts a 3:4:4 ratio for the three products they listed.

A small proportion of the students translated the line drawing for the starting material into a drawing that showed the positions of all the hydrogen atoms in this compound, as shown in Figure 4.

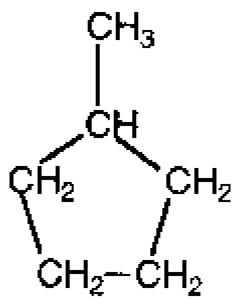

Figure 4. An alternate representation of the starting material drawn by every student who obtained the correct answer to this question.

All of the students who did this recognized that the reaction actually gives the four products shown in Figure 5.

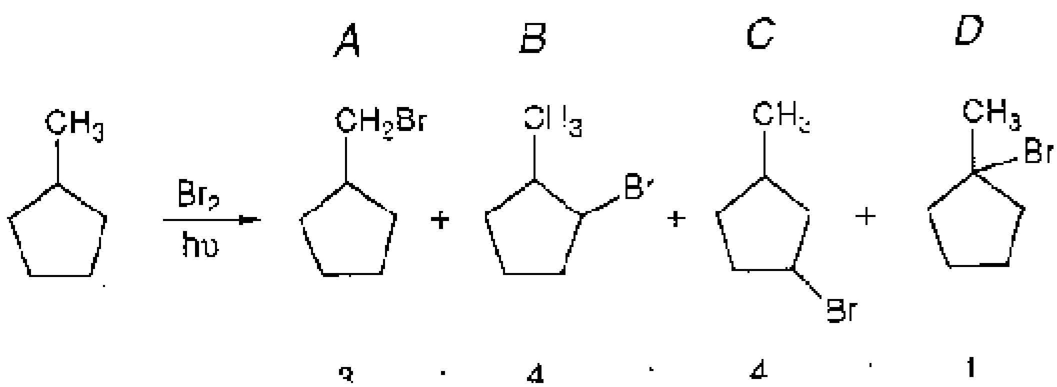

Figure 5. The accepted answer to this question.

These students also recognized that simple statistics would give a product distribution of 3:4:4:1. More importantly, these students came to the correct conclusion that it is the fourth product - the one their colleagues missed - that is the most likely product to be formed in this reaction because of the stability of the 3^{o} radical formed when the Br� radical attacks this carbon atom.

Before we can satisfy our goal of explaining the observations reported in this section we need to decide how the problem solving ability of various individuals should be compared and we need to define the term *representation*.

SUCCESSFUL VERSUS UNSUCCESSFUL PROBLEM SOLVERS

Efforts to understand the cognitive processes involved in problem solving have been underway for at least 100 years (Helmholtz, 1894). One approach has focused on differences between *expert* and *novice* problem solvers (Chi, Feltovich, & Glaser, 1981; Larkin, McDermott, Simon, & Simon, 1980; Schoenfeld & Herrmann, 1982). Smith (1992) has criticized this expert-novice dichotomy as unjustly equating expertise with success. He argued that "*successful* problem solvers often share more procedural characteristics that distinguish them from *unsuccessful* subjects than do experts when compared to novices (p. 182)."

We agree with those who argue that research on problem solving should focus on the differences between *successful* and *unsuccessful* problem solvers (Camacho & Good, 1989; Smith & Good, 1984). Our goal is a better understanding of the process by which individuals disembed relevant information from the statement of a problem and transform the problem into one they understand - in other words, how they build and manipulate the representation they construct of the problem. This paper pays particular attention to differences between both the number and kind of representations built by successful versus unsuccessful chemistry problem solvers and describes a theoretical model that offers a possible explanation for the role that representations play in determining the success or failure of the problem-solving process.

WHAT IS A REPRESENTATION?

The first step toward understanding the role that representations play in problem solving in any discipline involves building an adequate definition of what we mean by the term *representation*. Simon (1978) argued that the following is noncontroversial.

> The human brain encodes, modifies, and stores information that is received through its various sense organs, transforms that information by the process that is called 'thinking," and produces motor and verbal outputs of various kinds based on the stored information.

What is highly controversial, he concluded, is "*how* information is stored in the brain; in the usual terminology, how it is 'represented' ..."

Simon uses the term representation in the sense of an *internal* representation - information that has been encoded, modified, and stored in the brain. Martin (1982) uses the term in the same sense when he says that representations "signify our imperfect conceptions of the world."

Estes (1989) makes an important point when he reminds us that "a representation stands for but does not fully depict an item or event." He notes that representations are attempts the brain makes to encode experiences. Thus, a representation is very different from a photograph, which preserves all of the information in the scene - up to the resolving power of the film.

It is tempting to define an internal representation as the *mental image* that an object or event evokes in the individual who experiences it. Purists would note, however, that there is some question about whether representations can be stored as images (Pylyshyn, 1978). Within the context of research on problem solving, it is therefore useful to rely on an operational definition in which an internal representation is assumed to be the understanding an individual constructs about the problem being solved.

Greeno (1978, 1980) proposed three characteristics that can be used to evaluate a mental representation:

coherence, connectedness, and correspondence. A representation is *coherent* when it is internally consistent. It is *connected* when it is related to other concepts (or schema) the individual has constructed. *Correspondence* reflects the extent to which the representation is accurate because it matches reality. [Proponents of the constructivist theory of knowledge might prefer a definition in which correspondence is assumed to measure the extent to which the representation fits the knowledge shared among a community of scholars working in a particular field (Cobb, 1989).]

The modifier *internal* is added to the term representation to distinguish the information stored in the brain from *external representations*, which are physical manifestations of this information. An external representation can take the form of a sequence of words the individual uses to describe the information that resides in his or her mind. In other situations, it takes the form of a drawing or a list of information that captures particular elements of the mental representation. Within the context of problem solving in chemistry, it can include the equation - such as $PV = nRT$ or $E = E^o - RT/nF \ln Q$ - an individual writes that shapes the way information is processed in subsequent steps in the problem-solving process.

UNDERSTANDING THE PROBLEM: THE EARLY STAGES IN PROBLEM SOLVING

Ten years ago, we began a series of experiments to study the relationship between students' performance on tests of spatial ability and their performance on the hour exams they took while enrolled in college-level chemistry courses. We expected to find a correlation between students' performance on the spatial ability tests and their performance on exam questions that involved the manipulation of three-dimensional images. We found, however, that the magnitude of this correlation was equally strong for all questions that probed the students' problem-solving skills (Bodner & McMillen, 1986). Subsequent experiments with students in both general chemistry (Carter, LaRussa, & Bodner, 1987) and organic chemistry (Pribyl & Bodner, 1987) showed that correlations with tests of spatial ability were strongest for exam questions that differed significantly from those the students had seen previously. Regardless of the type of question that was asked, the tests of spatial ability correlated best with the student's performance on *novel problems*, rather than *routine exercises* (Bodner, 1991).

Because the spatial tests used in these experiments were tests of disembedding and cognitive restructuring in the spatial domain we concluded that there were preliminary stages in the problem-solving process that involved disembedding the relevant information from the statement of the problem and restructuring or transforming the problem into one the individual understands. We described the goal of the early stages of the problem-solving process as trying to *understand the problem* or to *find the problem*. Larkin (1985) reached similar conclusions when she concluded:

> To work on the problem, the solver must convert the string of words with which he is presented into some internal mental representation that can be manipulated in efforts to solve the problem. Understanding the problem then means constructing for it one of these internal representations.

The preliminary stages in the problem-solving process in which students begin to understand the problem can therefore be thought of as stages in which the first step is taken toward building a mental representation of the problem.

REPRESENTATION SYSTEMS

Whereas the work in general chemistry focused on multiple-choice exams, our study of the relationship between spatial ability and student performance in organic chemistry involved the analysis of answers to free-response questions, such as predicting the product of the following reaction (Pribyl & Bodner, 1987).

$PhCOOH + SOCl_2$ -->

Students who scored well on the tests of spatial ability were more likely to draw preliminary structures in which the "Ph" or phenyl group was represented by a six-member ring and the "COOH" carboxylic acid group was represented by an OH group attached to a C=O double bond. They were also more likely to score well on this question.

Students with low scores on the spatial tests were less likely to do well in the course and they were more likely to write equations such as:

$$PhCOOH + SOCl_2 \dashrightarrow PhCl + SO_2 + HCl$$

or:

$$PhCOOH + SOCl_2 \dashrightarrow PhCOOCl + SO_2 + HCl$$

In the first equation, a carbon and oxygen atom mysteriously disappear. With tongue firmly in cheek, we might suggest that the oxygen atom apparently crossed the room in which this test was taken to condense among the products of the second equation. It is important to recognize, however, that the most important characteristic of these equations is not the fact that they aren't balanced. (Organic chemists are notorious for writing equations that aren't balanced.) For our purposes, the important characteristic of these equations is the fact that they are "absurd" - they carry no resemblance to the physical reality of what can happen to the molecules involved in the reaction.

The results of our preliminary experiments on problem solving in organic chemistry were reinforced by the work that led to the observations summarized in the introduction. It seems that one of the differences between students who are successful in organic chemistry and those who are not appears to be their ability to switch from one representation system to another. Students who do poorly in organic chemistry often have difficulty escaping verbal/linguistic representation systems. They tend to handle chemical formulas and equations that involve these formulas in terms of letters and lines and numbers that aren't symbols because they don't represent or symbolize anything that has physical reality. Thus, they see nothing wrong with transforming PhCOOH into PhCl.

Students locked in a verbal/linguistic representation system can recognize that the verbal/linguistic representation on the left and the symbolic representation on the right in Figure 6 describe the same compound. But they aren't likely to spontaneously switch from the representation on the left to the one on the right, or vice versa. Other students - who tend to do better in the course - switch back and forth between these representation systems as needed.

$PhCO_2H$

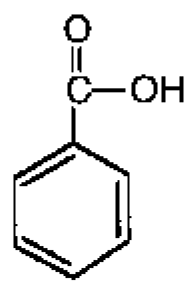

Figure 6. Verbal/linguistic and symbolic representations of benzoic acid.

If this hypothesis is correct, similar *external* representations might be written by individuals with very different *internal* representations. Consider the following equation, for example.

```
            O
           ||
CH3CH2CH2CCH3 + CH3MgBr  -->
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When they write this equation in their notebooks, students believe it is a direct copy of what the instructor writes on the blackboard. An observer, comparing the two, would agree that the students' notes seem to be direct copies of what the instructor wrote. In spite of the apparent similarity, there is a fundamental difference between what the instructor and many of the students write. The instructor writes *symbols*, which represent a physical reality. All too often, students write *letters and numbers and lines*, which have no physical meaning to them

Students for whom chemical formulas are examples of a verbal/linguistic representation system are more likely to write "absurd" formulas, such as the product shown in the following equation.

$$CH_3CH_2CH_2C(=O)CH_3 + CH_3MgBr \xrightarrow{Et_2O} CH_3CH_2CH_2C(=O)(CH_3)CH_3$$

It is only when the letters, numbers, and lines used to write these equations are symbols, which represent a physical reality, that students recognize why this answer is absurd or recognize the the flaw in the equation used to describe the graduate student's approach to the synthesis of a Grignard reagent.

DIFFERENCES IN THE NUMBER AND KIND OF REPRESENTATIONS CONSTRUCTED DURING PROBLEM SOLVING

As we have seen, an essential component of an individual's problem-solving behavior is the construction of a mental representation of the problem, which can contain elements of more than one representation system. We have therefore studied differences in both the number and types of representations constructed by successful and unsuccessful problem solvers among a population of 1st- and 2nd-year graduate students faced with questions that dealt with two-dimensional nuclear magnetic resonance spectroscopy (Domin & Bodner, in press).

Although they might not be familiar with the details of 2D-NMR, most readers will recognize that FT-NMR experiments involve irradiating the sample with a burst of RF energy, which is equivalent to exciting all the possible spin-state transitions at the same time. A detector then measures the change in the magnetization of the sample as it decays from saturation back to an equilibrium distribution of spin states. The signal collected from this experiment is subjected to a Fourier analysis, which transforms the signal from the time domain - in which it is collected - to a frequency domain spectrum identical to the result of the original NMR experiment.

2D-NMR is a two-dimensional NMR experiment that plays an important role in the process by which the individual peaks in the spectrum of a molecule are assigned to specific environments within the molecule. This content domain was chosen because multiple representations not only can but must be used to understand the 2D-NMR experiment. The data obtained in this study were consistent with the notion that the ability to switch between representations or representation systems plays an important role in determining success or failure in problem solving in chemistry. Successful problem solvers constructed significantly more representations than unsuccessful problem solvers.

The two groups also differed in the nature of the representations they constructed. Among the successful problem solvers, the most common representations were those that are best described as symbolic. These representations were characterized by a reliance on symbols or highly symbolic equations that might include fragments of a phrase or sentence. The most common representations constructed by the unsuccessful problem solvers were those best described as verbal. These representations, which were expressed either orally or in writing, contained intact sentences or phrases, such as: "the number of spin orientations of a spin-active nucleus is equal to two times the spin-quantum number plus one."

A THEORETICAL EXPLANATION OF THE DIFFERENCE BETWEEN SUCCESSFUL AND UNSUCCESSFUL PROBLEM SOLVERS

As you look back through this paper, you might recognize a theme that has dominated our work on problem solving, from our first experiments in general chemistry through our work with graduate students: *Successful problem solvers construct significantly more representations while solving a problem than those who aren't successful.*

Although our colleagues who teach organic chemistry are familiar enough with the content to successfully name the compound shown on the right in Figure 1 from the representation in which it was drawn, most of us would have to proceed the way the students who were successful on this task approached the problem. We would have to transform this Newman projection into a line structure, from which we could determine the name of the compound.

Our colleagues in organic chemistry would have no difficulty with the question based on Figure 2. For them, however, familiarity with similar tasks has transformed this question from a *problem* into a *routine exercise* (Bodner, 1987). Those of us for whom this task is still a problem would have to do what the successful students did, they would have to transform the starting material from the representation shown in Figure 2 into the one in Figure 4 - either within the minds or on the paper - before they could successfully answer the question.

Although the successful problem solvers throughout our work constructed significantly more representations than those who weren't successful, neither group constructed very many representations while solving the problems. In the 2D-NMR experiment, for example, the successful problem solvers constructed an average of about two representations per problem, while those who weren't successful constructed an average of just more than one representation per problem. A possible explanation for the difference between successful and unsuccessful problem solvers, which might provide insight into the role of mental representations in problem solving, can be found in the schema theory of cognitive structures. Schema theory views cognitive structure as a general knowledge structure used for understanding (Rumelhart & Ortony, 1977). Schema, also referred to as frames (Minsky, 1975) or scripts (Schank & Abelson, 1977), relate to one's general knowledge about the world. Schema are activated or triggered from an individual's perceptions of his or her environment and they provide the context on which general behaviors are based. Because they don't include information about any exact situation, the understanding of a situation they generate is incomplete. But, by including both facts about a *type of situation* and the *relationship* between these facts, they provide a structure that allows one to make inferences (Medin & Ross, 1992).

Within a given context, problem solving requires the activation of an appropriate schema that contains an algorithm or heuristic that guides the individual to the correct solution to the problem. The construction of the first representation is an effort by the individual to activate the appropriate schema. Thus, the first representation establishes a context for understanding the statement of the problem. In some cases, this representation contains enough information to both provide a context for the problem and to generate a solution to the problem. In other cases, additional representations may be needed since the solution may require more than one algorithm or heuristic. But the first representation provides the context in which the other representations are built.

Unsuccessful problem solvers seem to construct initial representations that activate an inappropriate schema for the problem. This can have three different consequences, each of which leads to an unsuccessful outcome: (1) the initial representation doesn't possess enough information to construct additional representations that contain algorithms or heuristics that might lead to the solution, and the individual gives up; (2) the initial representation leads to the construction of additional representations, but these representations activate inappropriate algorithms or heuristics, and eventually, an incorrect solution to the problem; or (3) the unsuccessful problem solver may never actually achieve an understanding of the problem, in spite of the number of representations that were constructed in an effort to establish a context for the problem.

IMPLICATIONS FOR THE TEACHING OF CHEMISTRY

Although most of our work on representation systems has focused on organic chemistry, a similar phenomenon exists in general chemistry. Perhaps the best way to illustrate this is to ask the reader to consider the following question: "Which weighs more, a liter of dry air at 25^{o}C and 1 atm, or a liter of air at this temperature and pressure that is saturated with water vapor? (Assume that the average molecular weight of air is 29.0 g/mol.)"

Most students (and some of their instructors) are convinced that air that has been saturated with water must weigh more than dry air. (It seems reasonable that adding water vapor to air must increase its weight.) Many of these individuals change their mind, however, when they are confronted with Figure 7.

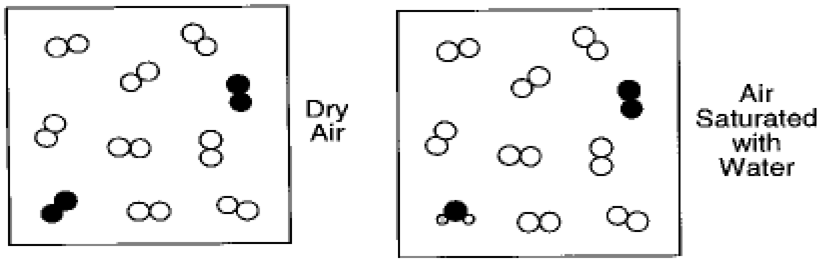


Figure 7. A symbolic representation of the difference between dry air and air saturated with water.

Figure 7 illustrates an important point: *Representations differ in the information they convey.* Encouraging students to use different representations when solving a problem might therefore simply be a way of helping them recognize what information is important in generating the answer to this question. The symbolic/pictorial representation in Figure 7 prompts us to consider the implications of Avogadro's hypothesis, which assumes that equal volumes of different gases contain the same number of particles. Because the molecular weight of water (18.015 g/mol) is significantly smaller than the average molecular weight of air (29.0 g/mol), water that has been saturated with air actually weighs less than dry air.

IMPLICATIONS FOR CHANGES IN HOW WE TEACH CHEMISTRY

One of the implications of this research on changes that might be made in the way we teach chemistry can be understood by considering what a typical beginning chemistry teacher would do if asked to work the following question in class: What is the pH of 100 mL of water to which one drop of 2 M HCl has been added?

The author's work with almost 1000 teaching assistants at the University of Illinois or Purdue University suggests that relatively few of these individuals would focus their approach to this problem around the drawing in Figure 8.

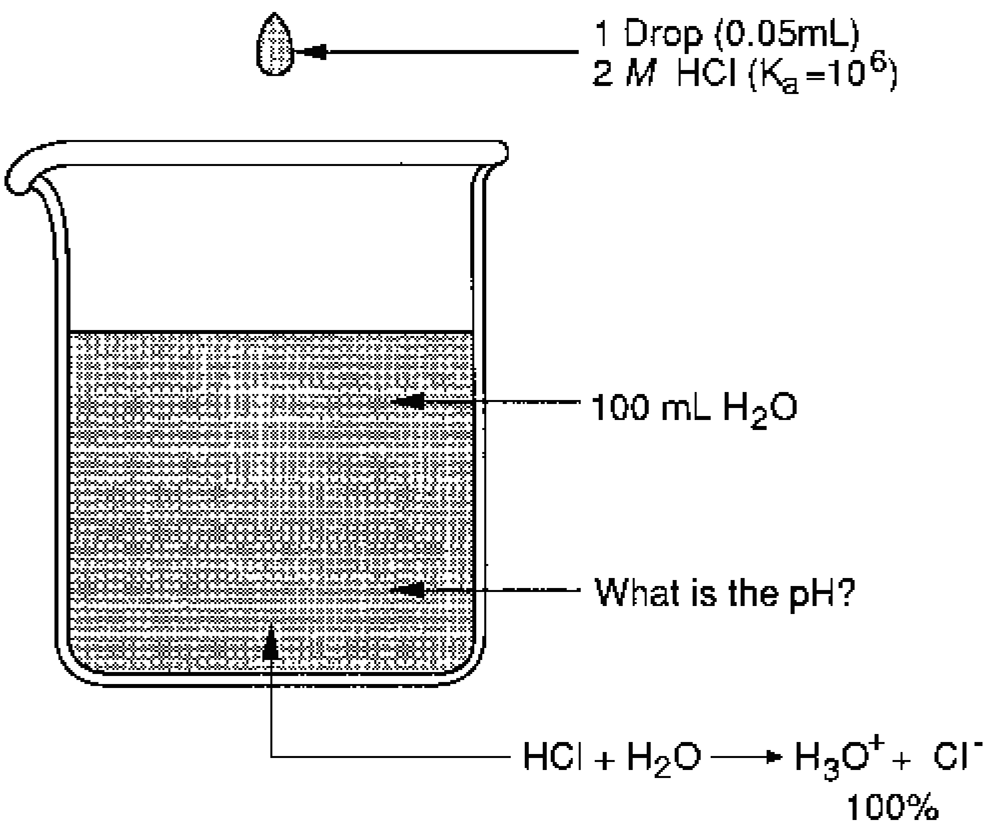


Figure 8.

This is important, because these individuals invariably focus their approach around a drawing when they encounter problems from other domains, such as the following question.

Two trains are stopped on adjacent tracks. The engine of one train is 1000 yards ahead of the engine of the other. The end of the caboose of the first train is 400 yards ahead of the end of the caboose of the other. The first train is three times as long as the second. How long are the trains?

It is important to recognize that Figure 8 isn't a drawing created before the problem is solved, but a drawing around which the solution of the problem is constructed. Each time more information is obtained - such as noting that a drop of this solution is about 0.05 mL or that HCl is a strong acid ($K_a = 10^6$) - it is incorporated into the drawing.

Most of those who read this paper won't be surprised to note that student performance on problem solving tasks improves when drawings of this nature are used when the instructor solves problem in class. They might be surprised, however, by another implication of the research described in this paper.

Imagine that you were trying to balance the following equation in class.

$I_3^- + S_2O_3^{2-} \text{-->} I^- + S_4O_6^{2-}$

Chemists have historically approached this task by separating the reaction into two components, balancing each half-reaction, and then combining the half-reactions.

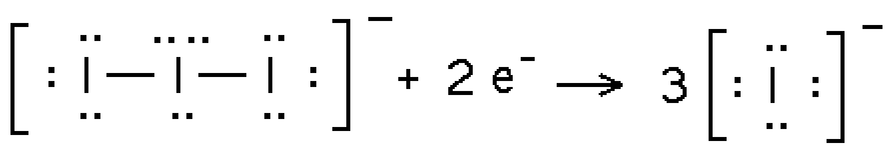
$I_3^- + 2\ e^- \text{-->} 3\ I^-$

$+\ 2\ S_2O_3^{2-} \text{-->} S_4O_6^{2-} + 2\ e^-$

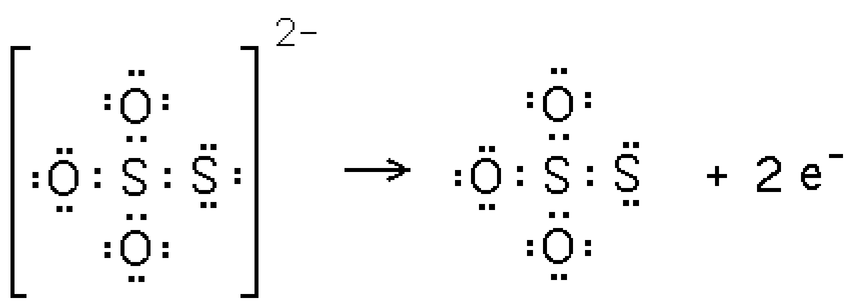
$I_3^- + 2\ S_2O_3^{2-} \text{-->} 3\ I^- + S_4O_6^{2-}$

When you listen to them talk about this in class, they utter statements such as: "Two electrons are added to the starting materials in the reduction half-reaction to *balance charge.*"

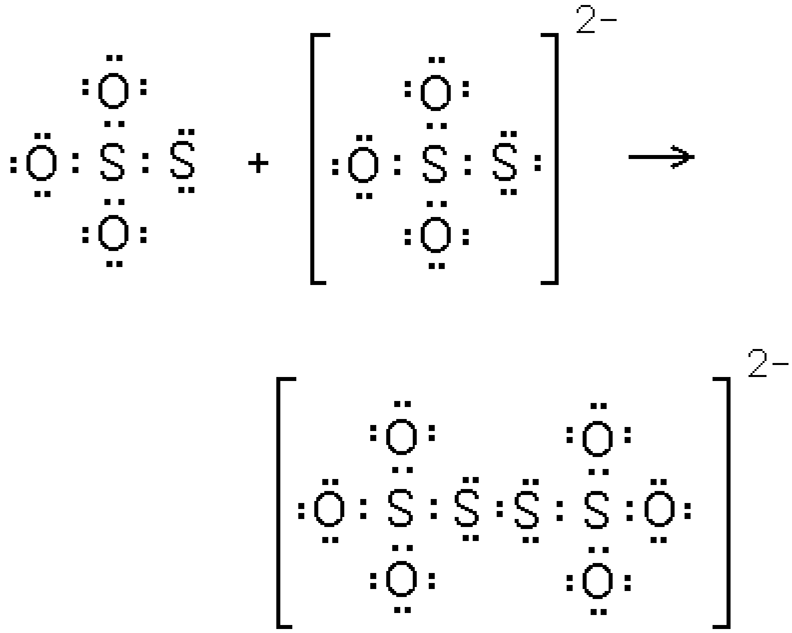
What would happen if the instructor approached this reaction using Lewis structures? Two electrons would no longer be added in the reduction half-reaction "to balance charge." They would be added to the system because two electrons are needed to transform the starting material into three iodide ions with filled octets of valence electrons.



Where are those electrons going to come from? They obviously have to come from the thiosulfate ion. And they are more likely to come from the terminal sulfur than from one of the oxygen atoms.



What happens to the neutral S_2O_3 molecule produced in this reaction? It combines with an $S_2O_3^{2-}$ ion to form an $S_4O_6^{2-}$ ion.



No one would argue that beginning students can use Lewis structures to predict the product of the two-electron oxidation of thiosulfate. We have evidence, however, that these students can understand how Lewis structures can be used to explain the product of this reaction. We also have evidence to suggest that students who have seen their instructor use this approach to balancing redox equations are more successful at similar tasks and more likely to understand what they are doing when they balance one of these equations. In many ways, this is nothing more than adding a symbolic representation - which carries different information - to the verbal/linguistic representation the students build when they read the equation they are being asked to balance.

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