Mental Models: The Role of Representations in Problem Solving in Chemistry

PROCEEDINGS

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A combination of techniques including field notes collected in operating classrooms, informal interviews with students in a tutorial environment, and formal structured interviews have been applied to study problem solving in chemistry among groups ranging from freshman enrolled in general chemistry through 6th-year graduate students within a variety of content domains including general, organic, inorganic, and physical chemistry. Regardless of the level of the students from whom data have been collected or the content domain in which the data were obtained we have found that one of the characteristic differences between successful and unsuccessful problem solvers is the number and kinds of representations they bring to the problem.

Introduction to Research on Problem Solving in Chemistry

For over 15 years, we have been interested in bridging the gap between theory and practice within the domain of problem solving in chemistry; a gap that results from fundamental differences between what chemists do when they solve problems and what they tell students to do when they teach problem solving, regardless of whether they are teaching secondary school students how to work stoichiometry problems or advanced graduate students how to synthesize natural products.

Any discussion of problem solving has to begin with a definition of the term ‘problem’,

Whenever there is a gap between where you are now and where you want to be, and you don’t know how to find a way to cross that gap, you have a problem.[1]

and the term ‘problem solving’.

Problem solving is what you do, when you don’t know what to do.[2]

These definitions have a logical consequence: there is a fundamental difference between tasks that are *routine exercises* and those that are *novel problems*. Some would argue that problems are more difficult, or more complex, than exercises. If they are right, it should be possible to devise a task that is intrinsically an exercise, or intrinsically a problem. Our work suggests they are wrong. The difference between an exercise and a problem is the result of differences in the level of familiarity with similar tasks the individual brings to a given task. Consider the following question, for example.

What weight of oxygen is required to burn 10.0 grams of magnesium?

$$2\ Mg(s) + O_2(g) \rightarrow 2\ MgO(s)$$

This question is a *routine exercise* for most chemists, who have done hundreds, if not thousands, of similar tasks. But it is a *novel problem* for beginning chemistry students.

More than 50 years ago, Polya proposed a model of problem solving that consists of four steps or stages.[3]

- Understand the problem
- Devise a plan
- Carry out the plan
- Look back

Our work suggests that this may be a model of what content specialists do when they work an *exercise* in their area of expertise; but it is not a model of the way people solve real problems. To probe this hypothesis, consider the following question set in a textbook[4].

A sample of a compound of xenon and fluorine was co~Æined in a bulb with a pressure of 24 torr. Hydrogen was added to the bulb until the pressure was 96 torr. Passage of an electric spark through the mixture produced Xe and HF. After the HF was removed by reaction with solid KOH, the final pressure of xenon and unreacted hydrogen in the bulb was 48 torr. What is the empirical formula of the xenon fluoride in the original sample?

When this problem is given to practicing chemists using a think-aloud protocol, it is clear that they do not follow Polya’s model by first understanding the problem, then devising a plan, and so on. The best evidence of this is the frequency with which they obtain an answer and then say: “Oh,... this is an empirical formula problem!” In other words, they only really understand the problem once it has been solved.

Several years ago, a more realistic model of problem solving was proposed by Grayson Wheatley. It consists of the following steps[5].

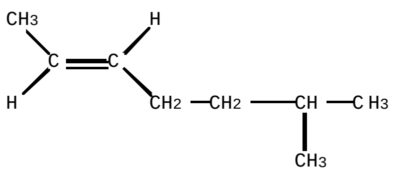
- Read the problem
- Now read the problem again
- Write down what you hope is the relevant information
- Draw a picture, make a list, or write an equation or formula to help you begin to understand the problem
- Try something
- Try something else
- See where this gets you
- Read the problem again
- Try something else
- See where this gets you
- Test intermediate results to see whether you are making any progress toward an answer

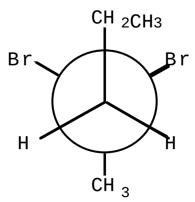
- Read the problem again
- When appropriate, strike your forehead and say, “son of a...”
- Write down ‘an’ answer (not necessarily ‘the’ answer)
- Test the answer to see if it makes sense
- Start over if you have to, celebrate if you don’t

Whereas exercises are worked in a linear, forward-chaining, rational manner, this model of problem solving is cyclic, reflective, and might appear irrational to someone watching us because it differs so much from the approach a subject matter expert would take to the task. The expert might be tempted to intervene, to show the ‘correct’ way of obtaining the answer. While this might make the expert feel good, it does not necessarily help the individual struggling with the problem.

Problem Solving in Non-mathematical Domains

Several years ago, students in the first-semester of an organic chemistry course for non-majors were given an exam in which they were asked to provide the systematic (IUPAC-approved) names of the following compounds:





Most of the students successfully named the compound on the left, but not the one on the right. The students were not much more successful at naming this compound when this part of the question was repeated on the next exam, or when it appeared on the final exam. The students’ success (or lack thereof) is not as interesting as their response to this question when they were interviewed after the exam. Time and time again, they complained that this part of the question was not ‘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 set the exam, the instructor (GMB) was convinced that this was a relatively easy question. (There is nothing wrong with the starting material, a common reagent used to prepare Grignard reagents. There is nothing wrong with the product of the reaction 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 potential source of H^+ ions that would destroy the Grignard reagent produced in this reaction, but many of them were unable to answer the question. When these students were interviewed after the exam, they frequently expressed the opinion that this was not a ‘fair’ question.

The reaction of methylcyclopentane with bromine provides a third example of a non-mathematical problem which students found difficult. The students were asked to predict the major products of the reaction, to estimate the ratio of these products that would be formed if bromine radicals were just as likely to attack one hydrogen atom as another, and to use the relative stability of alkyl radicals to predict which product was 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 three products, with a relative abundance of 3:2:2, as shown in Figure 1(a).

During interviews held with these students after the exam, we found that they recognized that attack by a bromine atom at any of the three hydrogen atoms in the CH_3 group would give the first product. They also recognized that the molecule is symmetric, 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.

Some of the students recognized that there are *two* hydrogen atoms on each of the carbon atoms at which attack occurs to give the second and third products in Figure 1(a). These students therefore recognized that simple statistics predicts a 3:4:4 ratio for these products. Without exception, these students recognized that the reaction actually gives four products, in a 3:4:4:1 ratio, as shown in Figure 1(b).

Every one of these students came to the correct conclusion that it is the fourth product – the one their colleagues missed – that is the most likely product of this reaction because of the stability of the tertiary radical formed when the bromine atom attacks this carbon atom.

For our purposes, however, the most important observation revolved around the difference between the behaviour of students who were successful on this question and those who were not. Every one of the students who gave the answer in Figure 1(b) did exactly the same thing: they 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 1(c). None of the students who gave the incorrect answer in Figure 1(a) did this.

Our colleagues who practice and teach organic chemistry would have no difficulty with these questions; they would treat them as routine exercises, whereas it is clear that for the students they are problems[6]. We suggest that what all three examples have in common is that the representations presented to the students do not contain sufficient information for the students to solve the problem. Students (and many professional chemists) are more familiar with line structures of molecules than with Newman projections. For this reason the first step in providing the systematic name for the molecule in Newman projection is to transform it into a line structure – a step which the experienced organic chemist finds unnecessary.

Figure 1a

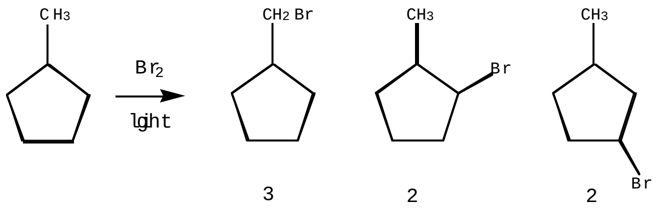


Figure 1b

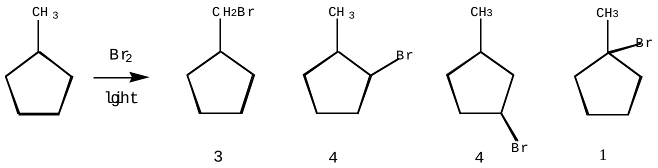
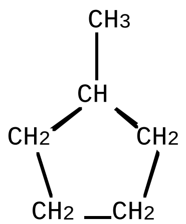


Figure 1c



The question based on the synthesis of a Grignard reagent causes no problems for our organic chemistry colleagues because the -OH group on the solvent would be a symbolic representation that would evoke images of protic solvents that would react rapidly (and perhaps violently) with the carbanion clearly evoked by the symbols 'CH_3CH_2MgBr'. The same is not true of students who either cannot or will not handle these letters and numbers as symbols for molecules or molecular fragments that can (and indeed will) undergo chemical reactions. Correct solutions to the third question, based on the reaction between methylcyclopentane and bromine, invariably involved the students in transforming the given representation as shown in Figure 1(c). This is a step which most experienced chemists would take automatically (either in their minds or on paper).

These examples hint that successful problem solving may involve the creation of appropriate representations. This suggestion requires more rigorous research and analysis. In order to do this 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[7]. One approach has focused on differences between 'expert' and 'novice' problem solvers[8-10]. Smith[11] 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.*"

We agree that research on problem solving should focus on the differences between successful and unsuccessful problem solvers[12,13]. Our goal is to achieve 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. We have therefore analyzed differences between both the number and the kind of representations built by successful and unsuccessful problem solvers in order to understand the role that representations play in determining the success or failure of the problem-solving process. The first step involves building an adequate definition of what we mean by the term 'representation'.

Simon[14] uses the term representation in the sense of an 'internal representation' – information that has been encoded, modified, and stored in the brain. Martin[15] uses the term in the same sense when he says that representations "*signify our imperfect conceptions of the world*." Estes[16] 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. Within the context of problem solving, it is useful to distinguish between internal and external representations. An operational definition of an internal representation is that it is the way in which the problem solver stores the internal components of the problem in his or her mind. In contrast to internal representations, 'external representations' are physical manifestations of this information. An external representation may be a sequence of words used to describe an internal representation, it may be a drawing or a list of information that captures particular elements of an internal representation, or (within the context of problem solving in chemistry) it can include the equation which shapes the way information is processed in subsequent steps in the problem-solving process – such as $PV = nRT$ or $E = E^{\circ} - RT/nF \ln Q$

Understanding the problem: The early stages in problem solving

Fifteen years ago, we began a series of experiments to study whether spatial ability is correlated with students' performance in the hour exams they took while enrolled in college-level chemistry courses[17]. Subsequent experiments with students in both general chemistry[18] and organic chemistry[19] 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 students' performance on *novel problems*, rather than *routine exercises*[6].

The tests of spatial ability used in these experiments were tests of disembedding and cognitive restructuring in the spatial domain. We therefore concluded that the 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 are particularly important in determining the success or failure of the problem-solving process. 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[20] reached similar conclusions when she concluded:

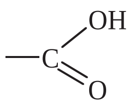
"To work on the problem, the solver must convert the string of words with which he is presented into some internal mental representation that can be manipulated in efforts to solve the problem. Understanding the problem then means constructing for it one of these internal representations."

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 an internal (or mental) representation of the problem.

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[18].

$$PhCOOH + SOCl_2 \rightarrow$$

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 carboxylic acid group was represented by



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:

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

or:

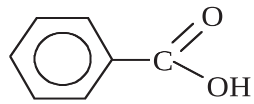
$$PhCOOH + SOCl_2 \rightarrow PhCOOCl + SO_2 + HCl$$

When these equations are shown to individuals who have many years of experience teaching general chemistry, they often note that the equations are not balanced. While this is true, it is not their most important characteristic (organic chemists are notorious for writing equations that are not balanced). For our purposes, the important characteristic of these equations is the fact that they are 'absurd' – there is no way to transform the starting materials into the products of these equations by the making and breaking of chemical bonds.

The correlation of success with spatial ability is consistent with our observations summarised earlier in this paper. We conclude that no matter how or where we collect data, we find that a significant difference between students who are successful in organic chemistry and those who are not is the students' ability to switch from one representation system to another.

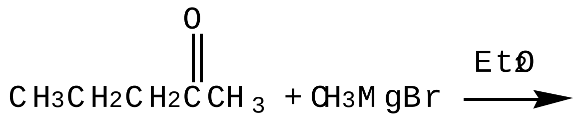
Interviews with students who do poorly in organic chemistry have shown that they often have difficulty escaping verbal/linguistic representation systems. They tend to handle chemical formulas and equations that involve these formulas in terms of letters and lines and numbers that cannot correctly be called symbols because they do not represent or symbolize anything that has physical reality. Thus, they see nothing wrong with transforming PhCOOH into PhCl. We believe this result is linked to previous work on students' inability or unwillingness to think of chemical systems in terms of the particulate nature of matter[21-29].

We have found that 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 (below) describe the same compound.

PhCOOH 

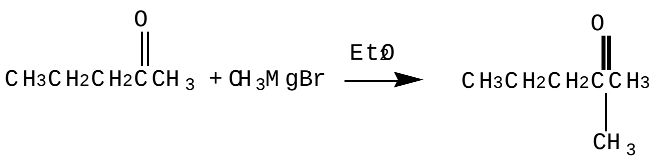
But they are unlikely to spontaneously switch from the representation on the left to the one on the right, or vice versa. Interviews with other students – who tend to do better in the course – have shown they switch back and forth between these representation systems as needed.

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



When they write this equation in their notebooks, students believe it is a direct copy of what the instructor writes on the blackboard. An objective observer, comparing the two, would conclude 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.

Interviews with students for whom chemical formulas are examples of a verbal/linguistic representation system showed that they are more likely to write 'absurd' formulas, such as the product shown in the following equation.



Only when the letters, numbers, and lines used to write these equations become symbols, representing a physical reality, do students recognize why this answer is absurd or recognize the flaw in the equation used to describe the graduate student's approach to the synthesis of a Grignard reagent described in the introduction.

The number and kind of representations constructed during problem solving

As we have seen, an essential component of an individual's problem-solving behaviour is the construction of a mental representation of the problem that 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 aspects of the FT-NMR experiment known as two-dimensional nuclear magnetic resonance spectroscopy[30].

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. This 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 complex 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 our study of students' success or failure at utilizing information in a computer tutorial on 2D-NMR 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[30]. Successful problem solvers constructed an average of about two representations per problem, while those who were unsuccessful constructed an average of just more than one representation per problem, a difference which is statistically significant.

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 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[31]. Schema, also referred to as frames[32] or scripts[33], 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 do not 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[34].

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 on 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.

- The initial representation does not possess enough information to generate additional representations that contain algorithms or heuristics that might lead to the solution, and the individual gives up.
- The initial representation leads to the construction of additional representations, but these representations activate inappropriate algorithms or heuristics and eventually lead to an incorrect solution to the problem.
- 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.

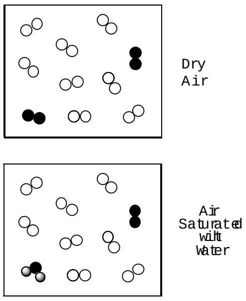
Implications for the teaching of chemistry

We have not yet completed a systematic study of what happens when our hypothesis about the role of multiple representations and multiple representation systems is used to change the way organic chemistry is taught in an operating classroom. We have, however, found that individual students, with whom we have worked in a one-to-one tutorial environment, can become more successful if we can convince them of the limitations of being trapped in a verbal/linguistic representation system.

Although most of our discussion of representations and representation systems so far 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 litre of dry air at 25ºC and 1 atm, or a litre of air at this temperature and pressure that is saturated with water vapour? (Assume that the average molecular weight of air is 29.0 g/mol.)*

Most students (and many of their instructors) are convinced that air saturated with water weighs more than dry air. (It seems reasonable that adding water vapour to air must increase its weight.) We have found, however, that many of these individuals change their mind when they are confronted with Figure 2.

Figure 2



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 2 prompts us to consider the implications of Avogadro's hypothesis, which assumes that equal volumes of different gases at the same temperature and pressure 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.

Another illustration of the implications of this research for changes that might be made in the way we teach chemistry is provided by the following question which a typical beginning chemistry teacher might put to a class:

What is the pH of 100 cm^3 of water to which one drop of 2 M HCl has been added?

The first author's work with almost 1000 teaching assistants at the University of Illinois or Purdue University suggests that relatively few of these individuals would instinctively focus their approach to this problem around the drawing in Figure 3. 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 from a placement exam given to students in the School of Science at Purdue University.

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?

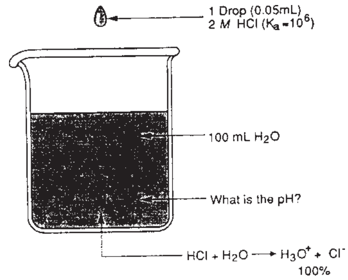
It is important to recognise that Figure 3 is not a drawing created *before* the problem is solved, but a drawing around which the solution of the problem is constructed. Each time more information is obtained – such as noting that a drop of this solution is about 0.05 cm^3 or that HCl is a strong acid ($K_a \approx 10^6$) – it is incorporated into the drawing. Most of those who read this paper will not be surprised to note that we have found 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.

$$I_3^-(aq) + S_2O_3^{2-}(aq) \rightarrow I^-(aq) + S_4O_6^{2-}(aq)$$

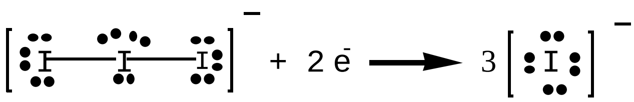
Chemists have historically approached this task by separating the reaction into two components, balancing each half-reaction, and then combining the half-reactions.

Figure 3

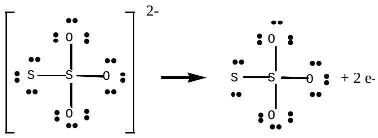


When you listen to them talk about this reaction in class, they utter statements such as: "two electrons are added to the starting materials in the reduction half-reaction *to balance charge*."

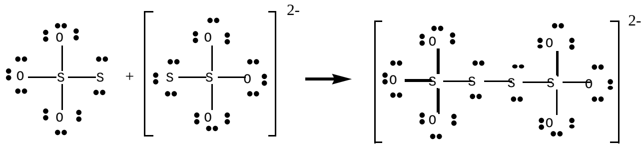
Recently, we have been teaching general chemistry by approaching reactions such as this in terms of Lewis structures. When this is done, two electrons are no longer added 'to balance charge'. They are added because two electrons are needed to transform the starting material into three iodide ions with filled octets of valence electrons.



These electrons obviously have to come from the thiosulfate ion. And they are more likely to come from the less electronegative terminal sulfur atom than one of the more electronegative oxygen atoms.



The neutral S_2O_3 molecule formed in this reaction combines with an $S_2O_3^{2-}$ ion to form the $S_4O_6^{2-}$ ion.



No one would argue that beginning students can use Lewis structures to *predict* the product of the reaction between the iodide ion and thiosulfate. We have preliminary evidence, however, that these students can understand how Lewis structures can be used to *explain* the products 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. Our goal is to develop an approach to descriptive chemistry that would enable at least some of the students who take general chemistry to *predict* the product of the reaction between ammonia and the hypochlorite ion, rather than memorizing that the Raschig process produces hydrazine.

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