College Chemistry Students’ Mental Models of Acids and Acid Strength
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Abstract: The central goal of this study was to characterize the mental models of acids and acid strength expressed by advanced college chemistry students when engaged in prediction, explanation, and justification tasks that asked them to rank chemical compounds based on their relative acid strength. For that purpose we completed a qualitative research study involving students enrolled in different types of organic chemistry course sections at our university. Our analysis led to the identification of four distinct mental models, some of which resembled scientific models of acids and acid strength. However, the distinct models are better characterized as synthetic models that combined assumptions from one or more scientific models with intuitive beliefs about factors that determine the properties of chemical substances. For many students in our sample, mental models served more as tools for heuristic decision-making based on intuitively appealing, but many times mistaken, concept associations rather than as cognitive tools to generate explanations. Although many research participants used a single general mental model to complete all of the interview tasks, the presence of specific problem features or changes in the nature of the task (e.g., prediction vs. explanation) prompted several students to change their mental model or to add a different mental representation. Our study indicates that properly diversifying and sequencing the types of academic tasks in which students are asked to participate could better foster meaningful learning as different types of cognitive resources may be activated by different students, and thus shared, analyzed, and discussed. © 2011 Wiley Periodicals, Inc. J Res Sci Teach 48: 396–413, 2011

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Research in science education in general, and in chemistry education in particular, at the college level over the past 30 years has been mostly focused on teaching and learning issues in introductory courses for science and engineering majors. Fewer studies have explored the nature and development of scientific knowledge and skills in advanced courses (Bodner & Weaver, 2008). This is problematic because our current understanding of how core concepts and ideas change or develop in a given discipline is mostly confined to those stages in which intuitive or naïve ways of conceptualizing the world are beginning to coexist with or be replaced by basic science constructs (Abell & Lederman, 2007). Little is known about how the understanding of these scientific concepts and ideas evolves with specialized training or how they are applied by more advanced students to make predictions or generate explanations when facing more complex questions and problems in their various disciplines.

The goal of the present study is thus to expand our knowledge base about college student understanding of central concepts in chemistry; in particular, their understanding of the concepts of acid and acid strength. For that purpose we completed a qualitative research study involving students enrolled in different types of organic chemistry course sections at our university. Our interest was to try to characterize the mental models expressed by these students when engaged in prototypical academic tasks that required them to make predictions and build explanations about the relative acid strength of different chemical substances. In particular, we wanted to identify the underlying assumptions on which these mental models were built, explore the influence that task content and task type had on the nature of the mental models that were expressed, as well as investigate how these models were used during different tasks.
Several authors have explored students’ ideas about a variety of acid–base chemistry topics using diverse research techniques (Carr, 1984; Cros et al., 1986; Drechsler & Schmidt, 2005; Lin & Chiu, 2007; Nakhleh, 1994; Ross & Munby, 1991). These studies have helped us build a good characterization of secondary school and introductory college chemistry students’ conceptions and mental models about the properties and behavior of acids and bases at the macroscopic and submicroscopic levels. In contrast, our understanding of advanced college chemistry students’ internal representations and reasoning in this area is rather sparse, with only a handful of published studies that have directly (Bhattacharyya, 2006) or indirectly (Ferguson & Bodner, 2008; Orgill & Sutherland, 2008) addressed the issue.

Our general interest in characterizing the predictive and explanatory models expressed by more advanced college chemistry students has several roots. On the one hand, we would like to better characterize the cognitive elements that guide and constrain these students’ reasoning while engaged in prototypical academic tasks. This knowledge is critical to devise support systems and instructional interventions that foster meaningful learning. On the other hand, we are interested in understanding how the particular characteristics of chemical theories and models affect student learning. These insights can help us enrich the pedagogical content knowledge of college chemistry instructors who traditionally do not have any formal educational training. In a broader sense, we are convinced that the results of our study have important implications for the teaching and learning of more specialized concepts and ideas in the various scientific disciplines.

Mental Models

One of the fundamental assumptions of modern cognitive science is that humans think about real and imaginary worlds through internal representations (Markman, 1999). Among the different kinds of representational structures that have been proposed, such as schemas and scripts, mental models have played a central role in different accounts of conceptual development and reasoning in scientific domains (Nersessian, 2008). In general, a mental model is conceived as a structural, behavioral, or functional analog of a real or imaginary object, process, event, or situation. Mental models are expected to support understanding, reasoning, and prediction in the situations in which they are involved, from logical reasoning in everyday situations to solving complex problems in knowledge-rich domains (Gentner, 2002).

Although research within the mental models framework is extensive and varied, a consensus view about issues such as the format of the mental models and the process involved in using them has not been reached among different research camps (Greca & Moreira, 2000; Nersessian, 2008). In the present work, mental models are conceived as dynamic internal representations that may be constructed on the spot to deal with the demands of a given problem or situation, although it is possible that in some cases mental models may be stored in long-term memory and deployed during a task (Gentner, 2002; Vosniadou, 1994, 2002). From this perspective, mental models may be unstable, inaccurate, inconsistent, and incomplete, and they may change continually as more information is noticed, acquired, or remembered. However, their construction or deployment is expected to be guided and constrained by the explicit and implicit cognitive resources available to any given individual (e.g., prior knowledge, ontological presuppositions, intuitive heuristics), as well as by the most salient features of the task at hand (Evans, 2006; Greca & Moreira, 2000; Osman & Stavy, 2006).

Mental model reasoning relies on qualitative relations, such as whether one quantity is greater or less than another (Gentner, 2002). Many of these relations represent causal rules that determine how the state of an entity will change as a result of changes of other elements (Chiou & Anderson, 2010; de Kleer & Brown, 1983). Thus, the elicitation of a mental model requires making explicit the nature of those entities and their assumed qualitative relationships (Vosniadou, 2002). Elicited mental models are often called “expressed” mental models as they are external representations of the target mental model as expressed through action, speech, writing, or any other material depiction and as interpreted by the researcher given the available evidence (Gilbert, Boulter, & Rutherford, 2000).

A variety of science education researchers have explored the expressed mental models of students as they engage in tasks involving diverse scientific concepts. In chemistry, these studies include investigations of students’ mental models of atoms and molecules (Harrison & Treagust, 1996), ionic bonding (Coll & Treagust, 2003), metallic bonding (Taber, 2003), chemical equilibrium (Chiu, Chou, & Liu, 2002), and acids and bases (Lin & Chiu, 2007). In this last study, Lin and Chiu (2007) identified four different mental models of acids and bases.
acids expressed by secondary school students; the use of these models depended on the nature of the task. Bhattacharyya (2006) investigated the mental models of acids expressed by organic chemistry graduate students while working on explanation tasks; this author identified one common mental model behind the reasoning of these students. Our work builds upon this research looking to characterize the mental models of acid and acid strength expressed by advanced college chemistry students as they engage in different types of activities (e.g., prediction, explanation, and justification). The results of our investigation provide insights on how these types of students use available cognitive resources to generate answers to relatively complex problems in which many potentially relevant factors need to be considered. They also highlight the influence that task content and type can have on the nature of the mental models that are used to build an answer.

Scientific Models of Acids and Acid Strength

To facilitate the description, analysis, and interpretation of the mental models expressed by participants in our study, it is useful to briefly discuss some of the basic characteristics of the scientific models developed to describe, predict, and explain the properties of acids. One of the major educational challenges associated with this topic is that chemists have developed a variety of models about acids and bases, which are often presented to students without much discussion of their underlying assumptions, range of application, and limitations (De Vos & Pilot, 2001; Furió-Máss, Calatayud, Guisasola, & Furió-Gómez, 2005). Thus, for example, at the macroscopic scale acids are described as substances or solutions that taste sour, corrode metals, and turn litmus paper red; in this context acid strength is determined by an acid’s ability to displace another acid from its salts (i.e., its reactivity with other substances). On the other hand, from a submicroscopic perspective acids are conceived in at least three different ways: the Arrhenius model, the Brønsted–Lowry model, and the Lewis model.

In the Arrhenius model, acids are thought of as substances that increase the concentration of hydrogen ions (H\(^+\)) when dissolved in water; acid strength is then determined by the extent to which a certain amount of the acid dissociates or reacts with water to produce H\(^+\) ions (Furió-Máss et al., 2005). In this context, “acidity” is traditionally conceived as an intrinsic property of a substance determined by its chemical composition and molecular structure. Although very useful in the characterization of the acid–base properties of many substances, the Arrhenius model has limitations, particularly in its inability to predict the behavior of chemical compounds in non-aqueous environments. The so-called Brønsted–Lowry model circumvents this limitation by proposing that acids are substances that contain ions or molecules than can donate protons (H\(^+\)) to other particles (called bases).

Acid strength in the Brønsted–Lowry approach should be conceived as an emerging property of a multiparticle system containing ions or molecules with acid–base properties. When we put an acid in a given solvent, acid particles are expected to donate protons to base (solvent) particles at a rate determined by specific composition and structural features of the ions or molecules involved. As a result of this proton transfer (forward process), new particles with acid–base properties will appear in the system (the so-called conjugate acid and base), which can also react with each other via proton transfer and regenerate the original particles (backward process). The extent of the acid–base reaction between the acid and the solvent, which is taken as the actual measure of acid strength, will thus be determined by the ratio of the forward to the backward reaction rates, which in turns depends on composition and structural features of all of the particles in the system. From this perspective, acid strength should be thought of as an extrinsic, rather than intrinsic, property of substances (i.e., it depends on the properties of both the substance and its environment). Thus, predictions of acid strength in the Brønsted–Lowry model can be made by carefully analyzing the electronic and steric effects that affect the reactivity of all of the particles involved. In particular, the best predictors happen to be those factors that either reduce electron charge density on the conjugate base, such as charge polarization via electrostatic induction (inductive effect) and electron delocalization (resonance), or strengthen intermolecular interactions with the solvent (e.g., molecular size and polarizability). Stabilization of the conjugate base reduces its rate of conversion to the acid form, increasing the extent of the overall reaction.

In a third submicroscopic description of acids and bases (Lewis model), acids are conceived as molecules or ions that can accept an electron pair during a chemical reaction, while bases are electron pair
donors. From this perspective, the hydrogen ion (H\(^{+}\)) that gets transferred in Brønsted–Lowry acid–base reactions is the Lewis acid itself, as this is the particle which accepts an electron pair from the reacting base. Acid strength in this model is also an emerging and extrinsic property of a substance that depends on the chemical nature of the Lewis acid, the solvent, and the products of the acid–base reaction. In general, factors that lead to stronger bonds between acid and base particles increase Lewis acid strength and predictions about relative values of this quantity can be made by analyzing composition and structural features of the acid ions or molecules (e.g., electronegativity and size of substituents on the acidic atom).

Methodology

Goals and Research Questions

The central goal of this study was to characterize the mental models of acids and acid strength expressed by college organic chemistry students when engaged in prediction, explanation, and justification tasks involving the ranking of chemical compounds based on their relative acid strength. In particular, our investigation was guided by the following research questions:

- What underlying assumptions about acids and acid strength characterize the mental models used by students to make predictions and build explanations?
- How does the nature of the task influence the mental models used to generate answers?
- How are these mental models used during different types of tasks?

Participants

The results of this study are based on data collected using semi-structured interviews of first-semester undergraduate organic chemistry students (\(n = 19\)) during the fall semesters of 2008 and 2009. The students were enrolled at a large, research intensive institution in the southwestern United States. First-semester organic chemistry students were chosen because they had already been exposed to the major theories and models of acid–base chemistry discussed at the college level and they could be expected to know how to apply them to the prediction and explanation of the chemical reactivity of organic substances. We recruited students from three different types of organic chemistry course sections: honors sections designed for the more advanced students (\(n_1 = 7\)), majors sections designed for students pursuing a bachelor’s degree in chemistry (\(n_2 = 6\)), and regular sections for other science and engineering majors (\(n_3 = 6\)). Participants only included students enrolled in college organic chemistry for the first time. Ten females and nine males volunteered to participate in our study. For reference and privacy purposes, a label was assigned to each of the participants based on their position on an interview list. For example, the third student on this list was assigned the label S3.

Research Instruments

We designed two analogous instruments (see Forms A and B in Figure 1) each divided into three main parts: prediction tasks, explanation task, and justification tasks. The inclusion of these three types of tasks created an opportunity for exploring students’ reasoning as applied to the most common questioning formats used to assess student understanding in chemistry (Dávila & Talanquer, 2010). To address validity and reliability issues, we asked experts in organic chemistry to review our research instruments and to provide feedback. Their comments and suggestions were used to build the final version of the questionnaires. Additionally, prior to data collection, a pilot study involving undergraduate and graduate students was completed to further evaluate the validity and reliability of each task and assess the interview protocol.

The first part of the research instruments included seven ranking tasks in which students were expected to predict the relative acid strength of a set of three different organic compounds represented by their skeletal structural formula (i.e., explicit cues about atomic composition and connectivity were visually available to the participants). Forms A and B of the instrument had four ranking tasks in common (tasks #3, #4, #5, and #7 in Figure 1) and three distinctive problems which allowed us to explore the effect of different structural factors on students’ thinking without making each of the questionnaires excessively long. Ranking tasks were chosen because they require students to make multiple inferences and decisions, and are commonly used in chemistry courses to elicit students’ ability to apply chemical models and principles in the prediction of a
variety of physical and chemical properties. Each of the ranking tasks was designed to assess students’ abilities to recognize important factors that determine acid strength (e.g., nature of the atom to which the acidic proton is attached, inductive effect, resonance). The set of three compounds included in each of the prediction tasks were chosen to generate questions with various levels of difficulty: Chemical substances in Figure 1.

Students were asked to (a) predict relative acid strengths in tasks #1 through #7, (b) explain trends in acid strength in task #8, and (c) justify their reasoning in ranking acid strength for the set of substances included in task #3, #6, and #7.

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questions one through three could be ranked by analyzing the effect of a single factor; acid strength for substances in questions four through six was determined by variations in two different factors, while the ranking of chemical compounds in question seven required the analysis of three variables.

The second part of the instruments included a single explanation task (questions #8A and #8B in Figure 1), in which students were expected to explain the trend in acid strength for a set of three (Form A) or four (Form B) chemical substances represented by their structural formula. Information about each of the substances’ $pK_a$ (a measure of acid strength) was explicitly provided. In the final part of the instrument, research participants were asked to justify their rankings for questions #3, #6, and #7. These three ranking tasks were chosen because they were judged to be the most complex among those questions requiring the analysis of one, two, or three factors, respectively, to predict acid strength. Results from a pilot study indicated that asking participants to generate justifications for each of the seven ranking tasks demanded excessive time and resulted in cognitive overload.

Data Collection

Students were randomly assigned to complete one of the two research instruments during the course of a 30-minute semi-structured interview (Greene, Caracelli, & Graham, 1989) conducted 1 or 2 weeks after formal instruction and assessment of the topic of acidity in their organic chemistry course. Data collection was approved by the Human Subjects Committee at our University; all of the participants consented to participate in the study. During the first part of the interview, each of the ranking tasks was shown one at a time on a laptop screen. Participants were asked to think out loud as they ranked the three chemical compounds from least to most acidic. Their responses were collected in written form using a worksheet and their verbal explanations were audio recorded. At this stage, students were told that they had 2 minutes to complete each task and they were not allowed to go back to previous problems once they advanced to the next set of substances. Our goal was to try to characterize students’ reasoning under speeded conditions and be able to compare it with that used in later parts of the interview. Upon completion of all of the ranking questions, students were asked to complete the explanation and justification tasks without any time constraints. All of the students’ productions during these latter stages, written or verbal, were also collected or audio recorded.

Data Analysis

All of the interviews were transcribed and carefully analyzed using an iterative, nonlinear constant comparison method in which common ideas, beliefs, prior knowledge, and reasoning strategies were identified within each task (Charmaz, 2006). Descriptive and interpretive codes were developed from the data set as a means to help answer each of the research questions. Although two similar forms of the instrument were used, transcripts corresponding to interviews based on Form A ($n_A = 9$) and Form B ($n_B = 10$) were analyzed using the same descriptive coding. During code interpretation, task responses were compared within and across types of forms.

An important part of the analysis was focused on the identification of explicit and implicit factors that interviewees used to predict, explain, or justify trends in acid strength. Given that the research instruments were designed to create opportunities for students to recognize important structural (e.g., specific type of atom attached to the acidic proton) and electronic (e.g., inductive effect, resonance) features that affect acid strength, these sets of factors were used to develop initial codes, which were then iteratively modified, collapsed, or expanded based on the analysis of all of the transcripts. Once a more complete and stable set of codes was generated, which included 35 different categories (e.g., presence of an –OH group; size of the molecule; bond type), transcripts were re-coded to ensure consistency in the analysis. Over 20% of the transcripts were coded by two different researchers using the same codebook (see Online Supplementary Materials) until inter-rater reliability was $>90%$.

Descriptive codes were used to generate a smaller set of interpretative codes summarizing general classes of features used by students to make predictions or build explanations or justifications during the interview tasks (e.g., presence of certain composition or structural features; stability of a molecule or parts of a molecule, resonance effect). These interpretative codes served as the basis for the inference process applied to characterize the assumptions that seemed to guide and constrain students’ reasoning about acids and acid strength while engaged in each specific problem and major type of task. For example, the consistent presence
of the interpretative code “resonance effect” in a student’s predictions about acid strength was frequently indicative of the underlying assumption: Strong acids are proton donors that have a stable conjugate base. Other examples of how this part of the analysis was completed are presented in the Online Supplementary Materials associated with this paper.

Identification of differences and similarities among explicit and implicit assumptions about acids and acid strength allowed us to generate a first description of different classes of mental models expressed by our study participants. Expressed mental models were characterized by the set of assumptions that a student seemed to use to guide her or his thinking during specific problems or major types of tasks; this allowed us to detect changes or shifts in mental models at specific points during the interview. Initial model descriptions were then used by two researchers to independently classify students in different groups based on the nature of their expressed mental models of acidity. An iterative process of comparison, discussion, and redefinition of the core assumptions underlying each mental model, as well as of the placement of each participant in a given group, led to the major findings summarized in the following section.

Findings

Our analysis led to the identification of four distinct mental models of acid and acid strength (Models A, B, C, and D in Table 1) expressed by our research participants while engaged in the different interview tasks. However, Model D was only expressed in conjunction with one or more of the other models. It is important to point out that we decided to differentiate mental models based on differences in general, rather than specific, assumptions about what makes a substance an acid and what factors determine acid strength. For example, if a student thought of acids as substances that had oxygen, with acid strength determined by the number of

### Table 1

**Underlying assumptions associated with the different mental models of acid and acid strength expressed by research participants in the present study**

<table>
<thead>
<tr>
<th>Model Type</th>
<th>Participants&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Single Model</th>
<th>Multiple Models: Feature-Triggered, Nature of the Problem Induces Model Change or Addition</th>
<th>Multiple Models: Task-Triggered, Nature of the Task Induces Model Change or Addition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model A: Acidity as an intrinsic property of substances. Acid strength determined by the presence of certain types of atoms or functional groups in the molecule (composition/structural features). Lack, or very underdeveloped, sense of mechanism for acid behavior. Acids perceived as unstable substances</td>
<td>S3 (R), S9 (R), S11 (H), S15 (H), S16 (M)</td>
<td></td>
<td>S10 (R), S18 (H)</td>
<td></td>
</tr>
<tr>
<td>Model B: Acids as substances that lose hydrogens or protons. Acid strength determined by intrinsic properties of the acid, some explicit (# of H atoms) some implicit (polarity), some molecular (molecular polarity), some local (bond polarity)</td>
<td>S2 (M), S17 (M)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model C: Acids as substances that donate protons. Acid strength determined by implicit properties of the molecule (mostly electronic; mostly local) that help stabilize the conjugate base</td>
<td>S5 (M), S13 (H), S14 (H), S19 (H)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model D: Acids as substances that accept electrons. Acid strength determined by number of lone electron pairs or empty orbitals</td>
<td></td>
<td>S12 (H)</td>
<td>S4 (R)</td>
<td></td>
</tr>
</tbody>
</table>

The table shows the distribution of participants based on their expressed mental model(s).

<sup>a</sup>Participants were enrolled in course sections designed for regular (R), chemistry major (M), or honors (H) students.
oxygen atoms in the system, while another student thought of acids as substances that contained hydrogen, with acid strength determined by the relative position of these hydrogen atoms in the molecule, they would have been classified as expressing a similar mental model based on general assumptions such as: Acidity is an intrinsic property of substances; acid strength is determined by the presence of certain types of atoms or atomic arrangements in the acid’s molecules (composition/structure features). It was considered that the differentiation at this general level captured the core, and most educationally relevant differences in our participants’ reasoning. From this perspective, the following paragraphs describe our own conceptualization of the mental models of acid and acid strength expressed by the interviewees based on the analysis of the data through this more general lens.

Our results indicate that over a half of the students (11/19) relied on a single general mental model to reason through the prediction, explanation, and justification tasks, but several of them (8/19) changed or added assumptions from different mental models as a result of the engagement with a new problem or a new type of task. All of the latter students are classified as “Multiple Models” in Table 1 but they are divided into two major groups, feature-triggered and task-triggered, based on the context that led to the expression of different mental models during the interview. Students classified as “feature-triggered” mostly relied on one mental model to make decisions about acid strength but used criteria from a different model to make these types of judgments in a few of the ranking problems. Our analysis suggested that model revision in these cases was triggered by the identification of specific composition or structural features of the substances included in a given question. On the other hand, participants identified as “task-triggered” relied on a single mental model to make predictions about acid strength across different problems, but drastically changed their expressed mental model or added a new mental model as a result of the engagement in the explanation or the justification tasks. Our analysis suggested that model change or addition in these cases was related to recalling or recognizing additional factors that influence acid strength as students tried to make sense of the data included in the explanation task (question #8 in Table 1). As shown in Table 1, there is no clear differentiation between the mental models expressed by students enrolled in course sections designed for regular (R), chemistry major (M), or honors (H) students.

Given the size of our sample, we cannot claim to have developed an exhaustive characterization of the mental models and reasoning patterns that college organic chemistry students may express while working on similar prediction, explanation, and justification tasks. However, our results illustrate the wide variety of mental models and reasoning patterns expressed by college students at similar points in their training as science or engineering majors, as well as some of the common assumptions that seemed to guide and constrain their reasoning about acids and acid strength. Nor do we intend to assert that the mental models described in the following paragraphs correspond to robust cognitive representations in the long-term memory of our interviewees. Our analysis and description tried to capture the functional mental models generated or deployed by our research participants while engaged in specific tasks in a particular context. However, one can speculate about the strength or robustness of these representations based on the consistency and coherence with which they were applied. In our study, judgments about the strength of different assumptions were based on the analysis of the extent to which they were systematically applied across different contexts (diSessa, 2004). In particular, students’ assumptions were deemed “weak” if they were applied inconsistently or in a contradictory manner across ranking problems or between prediction, explanation, and justification tasks.

Mental Model A

A significant fraction of our interviewees (7/19) expressed a rather underdeveloped conceptualization of acids and acid strength; five of these participants relied on this way of thinking across the entire interview. For people in this group, “acidity” seemed to be an intrinsic property of some substances determined by the presence of certain atoms or functional groups that were acidic or basic by nature (composition/structure features). To illustrate these ideas, let us consider the following interview excerpt:

S9: Mmm. Okay, so they all have the ring and the double bond O and then OH. Okay, I believe OH is more basic. I’m gonna say B is the least acidic... I don’t really think of oxygen as being acidic, so maybe C would be the middle one and then A would be the most acidic.
Int: So, why don’t you think of oxygen as being acidic?
S9: Because it’s so abundant, and we breathe it. So, maybe it would be hard for it to be acidic, I think.
(S9 working on question #6A in Figure 1)

As exemplified by this excerpt, students who used Mental Model A thought of certain atoms, such as H, O, or Cl, or certain functional groups, such as hydroxyl (–OH) or carbonyl (–C=O), as intrinsically acidic or basic, and seemed to assume that these properties were “inherited” by the chemical compound in which these composition or structural features were present.

Students in this group lacked or had a very underdeveloped sense of mechanism for acid–base behavior at the molecular level. Acid strength was predicted or explained based on the mere presence, or absence, of some components or by paying attention to the relative number of these composition or structural features in different molecules, relying on heuristics of the form “More A–More B” (Stavy & Tirosh, 2000; Maeyer & Talanquer, 2010) to make the final decision:

Okay, I’m gonna say C is the least acidic because it’s different than A and B. A is basically B doubled, so maybe A is the most acidic? (S9 working on question #4)

In a few instances students referred to some atoms or functional groups, or to the entire molecule, as having some implicit property (e.g., electronegativity, polarity) that made them acidic or basic but without understanding how or why. In these cases, heuristic reasoning was also applied to complete the tasks (e.g., the more polar the molecule, the more acidic). Four students in this group expressed the belief that acid behavior was somewhat related to the “stability” of the molecule; in particular, the assumption that acids were unstable substances was predominant in some cases. These beliefs allowed some students to generate simple mechanistic explanations for differences in acid strength based on the idea that uneven distributions of charge (as caused by the presence of certain atoms or functional groups, or by their relative positions) induced molecular instability.

Many of the ideas or beliefs expressed by this group of students were rather weak in the sense that they changed from one ranking task to the other, or between prediction, explanation, and justification tasks. Consider, for example, S9’s ideas about the “acidic” nature of hydrogen while working on question #2A:

It just seems like hydrogen usually doesn’t play much in the like acidity thing... Okay, I’m gonna guess the more chlorine the more acidic.

compared to her thinking while justifying her answer to question #7:

Yea, maybe the Hs have something to do with acidity... I’m not sure. Now that I think about it, I think that the Hs might be acidic... So, maybe B would be the most acidic. Oh, that’s what I wrote! I’d go with that.

In many cases, it was difficult to identify which features of a task triggered a change in ideas or beliefs, beyond the fact that the modification allowed students to better differentiate between substances or further justify their predictions.

**Mental Model B**

Students who expressed Mental Model B thought of acids as substances that could lose hydrogen atoms or protons (H⁺). This assumption guided their reasoning about acid strength as they identified or looked for factors that could explain why some compounds lost more of these particles, or lost them more easily. However, all of the factors that they considered were explicit or implicit features of the represented acids, with no reference to the effect of conjugate base stability on acid strength. This suggests that although students in this group seemed to have developed a powerful assumption for reasoning about acids (i.e., acids lose H or H⁺), they still thought of acidic behavior as an intrinsic property of some chemical compounds solely
determined by specific composition or structural features of the acid form (as seen in students who expressed Mental Model A).

The number and diversity of factors considered by students who relied on Mental Model B in making decisions about acid strength varied at points during the interview (S2 and S17, who used Mental Model B across all of the tasks; S10 and S18, who relied on this model only during the explanation and justification tasks; Table 1). Consider, for example, these excerpts from the interview with S17 as this student worked on two different ranking tasks:

In terms of acidity, I would vote A most acidic because the hydrogen is farthest away from the chlorine. It has the most freedom to bond with whatever it chooses. (S17 working on question #2B)

... C has the methyl attached to it which means it has more hydrogens. So, I’m going to vote C as the most acidic. (S17 working on question #6B)

This student considered all of the following explicit and implicit features in making decisions about acid strength: bond strength, bond length, number of hydrogen atoms in a molecule, relative position of some atoms in a molecule, perceived stability of a molecule, and atomic size. In general, the choice of decision-making cues seemed to be determined by the most salient feature in a given ranking task (e.g., presence of single, double, and triple bonds in question #1B; number of hydrogen atoms in a substituent in questions #4B, #5B, #6B, and #7B). Contrast this way of reasoning with that of research participant S10, who consistently relied on the following single assumption in the application of Mental Model B across the explanation and justification tasks: the more polar the molecule the easier for it to lose a proton (H⁺).

Some students in this group struggled to consistently apply their criteria for determining acid strength. For example, S2 based most of his judgments about acid strength on the perceived polarity of bonds, functional groups, or entire molecules which he inferred from the electronegativity of the atoms involved. The type of polarity (bond, group, or molecular) that he considered for decision-making varied from task to task, as well as his stated beliefs about the relationship between polarity and acid strength. In some cases, this student thought that the more polar an entity (bond, functional group, molecule) the easier for it to lose the proton:

For this one, I think it has something to do with the OH groups... It wants to donate a proton easier because they’re polar and can give it off better. (S2 working on question #3)

In other cases, the student thought that polar entities may better hold on to the hydrogen atoms and thus non-polar groups would be more acidic:

I’m trying to see how it would lose the H, which one it would be easier to lose the H on. Because if it’s non polar then, well mostly non polar, I think it would have an easier time losing the H but I’m not sure. I’m just gonna go with that. (S2 working on question #7A)

Although the student was aware of his contradictory reasoning while working on the different tasks, he was unable to resolve the inconsistency during the interview. He applied one or the other criterion depending on the structural features of a molecule that were more salient to him in a given task. This pattern of reasoning, in which students applied contradictory reasoning from one task to another, showing clear signs of awareness of the conflict, but without resolving the issue or selecting one option over the other, was common among several of our interviewees independent of the general mental model that they expressed.

In general, although students in this group had a much more developed sense of mechanism for acid behavior, or could more easily propose plausible mechanisms on the spot to justify their decisions than students who only expressed Mental Model A, their reasoning often relied on incorrect or incomplete representations of the relationships between composition, structural, and electronic features in a molecule and its acid strength. Thus, in many instances their mental model served more as a tool for
heuristic decision-making based on intuitively appealing, but many times mistaken, “More A—More B” associations (e.g., the more hydrogen atoms in the molecule, the more easily it will lose them; the more polar a molecule is, the easier for it to lose protons), rather than as a cognitive tool to generate explanations.

**Mental Model C**

For students who expressed Mental Model C (Table 1), acids were substances that lose or donate protons (H\(^+\)) and thus became charged after H\(^+\) ions were removed. In contrast with the two previous mental models, in which acid strength was thought of as only determined by explicit or implicit properties of the acid form of a given molecule (as represented in the research instrument), students that relied on this mental model based their predictions of acid strength on the presence of implicit molecular features (mostly electronic) that helped stabilize the charge on the conjugate base: the product of proton dissociation. In this sense, these students expressed a general mental model that was similar to the scientific model for Brønsted–Lowry acids, although we do not have enough data to evaluate to what extent they actually thought of acid strength as an extrinsic property of chemical substances determined by molecular features of both the acid and its conjugate base, as well as by the chemical nature of their environment.

In general, students in this group relied on the identification of electronegative substituents, double bonds between atoms, and conjugate systems in the different molecules to make decisions about the potential stability of the conjugate base. The common trend was to look for factors that could “stabilize” the extra charge once an H\(^+\) ion was lost or donated. However, there were significant differences in the ability of these research participants to explain how different features affected molecular stability, for example, a student like S13 did not clearly differentiate between stabilization via electrostatic induction (inductive effect) versus stabilization via electron delocalization (resonance). Consider the following interview excerpts as this student worked on two different ranking tasks:

So, if I have Cl. So, here it looks like it’s asking for inductive effect. This chlorine’s electronegativity is going to help delocalize the electrons . . . (S13 working on question #2B)

OK, so I think is going to go B, C, A because fluorine is more electronegative so it’s going to help with the delocalization and pull electrons away from the acidic proton. (S13 working on question #5)

Other students, like S19, could recognize most of the electronic factors that affected acid strength but were unable to provide a mechanistic explanation for their effects:

S19: OK, I said B was the most acidic because it’s aromatic, um because it provides more resonance structures.

Int: How does more resonance structures affect acidity?

S19: More resonance structures stabilize the negative charge that would result.

Int: How does it stabilize it?

S19: That’s a good question (laughs). It’s probably been explained, but I don’t know. (S19 justifying the answer for question #3)

The lack of a clear understanding of how resonance helps stabilize the conjugate base may have been responsible for these students’ consistent reliance on the reasoning heuristic “the more resonance structures, the more stable the conjugate base” to make decisions about acid strength, regardless of the relative stability of the different resonance forms. Similarly, the failure to understand how electrostatic induction can stabilize or destabilize a negative charge may explain why none of these students could recognize the effect of the more electropositive substituents (e.g., –CH\(_3\) group) on acid strength. In general, students in this group seemed to have built very strong associations between conjugate base stability and both electron charge delocalization and electron charge pulling by electronegative atoms in a molecule, but without meaningful understanding about how these phenomena caused stabilization. We did not find evidence that these students realized that factors that decreased local electron charge density around the acidic site would stabilize the conjugate base (e.g., electron delocalization), while those that increased it (e.g., electropositive substituents) would destabilize the conjugate base.
Despite their inability to generate complete explanations or justifications for their decisions, students who only expressed Mental Model C exhibited a significantly higher level of performance in the ranking tasks (57% average score) than any of the other groups of students, all of which performed at a comparably lower level (~35% average score). This indicates that Mental Model C was a better guide in the identification and selection of cues that were relevant for making decisions about acid strength. Compared to other groups of students, these participants were more coherent and consistent in their application of comparison criteria across different ranking problems and major types of tasks. This suggests that they had developed a more robust mental representation about acids and acid strength.

**Mental Model D**

Two of the participants in our research study (S4 and S12 in Table 1) conceived acids as chemical compounds that accepted electrons (Mental Model D), resembling the concept of a Lewis acid. When expressing this mental model, students thought of acid strength as determined by (a) the number of lone electron pairs in a molecule, (b) the “concentration” of electrons or negative charge as induced by the presence of electronegative atoms, or (c) the presence of empty orbitals that could accommodate more electrons. The underlying assumptions seemed to be that the more electrons, or the greater the electron density in the system, the weaker the acid because the molecule would be either less likely to accept more electrons or could accept hydrogens (behave like a base). To illustrate these ideas, consider the following interview excerpts:

OK we got fluorine on A, hydrogen on B, and chlorine on C. We know that fluorine is more electronegative than the other two. Chlorine is obviously more electronegative than H₂. Electronegative means it has the ability to attract more electrons, which means is going to be more basic. Least acidic is going to be the most electronegative. So, it’s going to be ACB. (S4 working on question #5; final ranking A < C < B)

Least acidic to most acidic . . . here I have two lone pairs of electrons and here I have four and here I have two. And I have here, I have a, well an H and I’m just gonna decide based on the number of lone pairs of electrons . . . So, I’m thinking that the more electrons—the more lone pairs of electrons present, then the harder it would be to get more electrons (S12 working on question #4; final ranking A < B < C).

The latter interview excerpt shows how S12 used Mental Model D to select A as the least acidic substance (molecule A has two oxygen atoms, with two lone electron pairs each; see question #4 in Figure 1), but applied Mental Model B to choose C as the most acidic compound because of the presence of an explicit hydrogen on its structural formula. This highlights the finding that participants in our study who expressed Mental Model D did it in conjunction with other mental models, and thus they are better characterized as “Multiple Model” thinkers, either feature-triggered (S12) or task-triggered (S4).

**Multiple Models: Feature-Triggered**

Some of our study participants (4/19) expressed more than one mental model throughout the interview and changes in their mental representations seemed to be triggered by the presence of specific composition or structural features in the substances included in the different ranking tasks. In general, most of these students thought of acids as substances that lost hydrogen atoms or protons and associated acid strength with explicit (e.g., # of hydrogen atoms in the molecule, # of double bonds) and implicit (e.g., electronegativity, bond and molecular polarity, bond length, atomic size, hybridization) features of the represented acid (Mental Model B). However, in some ranking problems they considered implicit properties of the conjugate base (e.g., resonance, ion stability) to make their decisions (Mental Model C). On average, these research participants used a wider variety of cues to make ranking decisions than students that expressed a single mental model and thus often struggled to select the relevant factors that affected acid strength.

For this set of students perceived differences in the electronegativity or size of the atoms present in a set of molecules tended to trigger the expression of Mental Model B while perceived differences in degrees of
unsaturation or conjugation led to the expression of Mental Model C. In the first case, increasing acid strength was often associated with the weakening of a chemical bond by either the pulling of electrons from the acidic proton by a more electronegative atom (or a more polar molecule), or the increased distance between the proton and a larger atom. The following interview excerpt illustrates these types of reasoning:

Um, for most acidic I guess that the sulfur and cesium would both be more acidic than water because they both have larger atomic radii (or)es which would mean they hold onto the hydrogens less than the oxygen which would hold on to them closer. (S7 working on question #1A)

On the other hand, the presence of double bonds or conjugated systems (e.g., benzyl group) in a molecule often prompted these students to justify their decisions considering the potential stability of the conjugate base, rather than solely based on composition and structural characteristics of the acid. Some students made very explicit the perceived difference in the nature of these questions. Consider the following excerpt from S20’s interview after this student finished question #2A (in which ranking decisions were based on “electron pulling” arguments) and started to work on question #3:

This is a different thing altogether, but I’m pretty sure B is gonna be the most acidic. Well, for one reason, it’s really, really stable. It has all these multiple resonance forms . . . you’ve got this benzene ring which basically is these two resonance forms that when you put them together are ridiculously stable. So, on that one, the stability makes it more acidic. Because it means that once the hydrogen comes off, what’s remaining is also really stable.

As also illustrated by the former interview excerpt, students in this group often referred to the stability of the acid to justify their reasoning. However, their ideas about the effect of such stability was varied, with some students claiming that the more stable the acid, the stronger it would be (better at responding to changes), while others thought that acid instability favored losing hydrogens or protons (more reactive molecule). Despite the commonalities in their expressed mental models, participants in this group varied widely in the frequency and consistency with which they relied on relevant (e.g., size and electronegativity of the atoms attached to the acidic hydrogen) versus irrelevant (e.g., # of hydrogen atoms in the molecule) features to make their decisions. They also differed significantly in their ability to generate mechanistic explanations and justifications. These latter tasks allowed them to expand and revise their ideas, but no major changes were observed in their core reasoning assumptions.

Among the students in this group, S12 stands out because he expressed three different mental models while working in the interview tasks. The presence of specific composition or structural features in the representations of the set of substances to be ranked had a strong influence on this student’s decisions across all of the tasks. For example, the presence of a benzene ring triggered predictions and explanations based on substance stability gained through resonance (Mental Model C); the existence of different numbers of atoms with lone electron pairs focused his attention on the ability of the system to accept or donate electrons (Mental Model D), while the presence of hydrogen atoms was used to select the stronger acid in other tasks (Mental Model B). Which of the models was dominant in guiding his reasoning seemed to be determined by those explicit salient features of a given task that allowed him to differentiate one substance from another.

Multiple Models: Task-Triggered

For most of our research participants, the explanation and justification tasks served as an “anchor” to (a) reaffirm ideas, as the observed trends in acid strength matched their expectations, (b) modify beliefs, as the trends did not correspond to their predictions, and (c) introduce new ideas, as some explicit or implicit features not noticed before could now be associated with a particular trend. However, in four cases (S4, S6, S10, S18; see Table 1) the explanation or the justification task triggered a “shift” in student reasoning as these interviewees seemed to either switch from one mental model to another to guide their thinking (S6, S10, S18) or add a different mental model to explain and justify their decisions (S4). In particular, students’ struggle with the meaning of the $pK_a$ values shown in the explanation tasks (questions #8A and #8B in Figure 1) seemed to serve as a trigger for prior knowledge that students had not activated up to that point.

Journal of Research in Science Teaching
Research participants S10 and S18 experienced the most drastic mental model shift, changing from consistently expressing Mental Model A throughout the prediction task, to fully basing their explanation and justifications on Mental Model B. In these two cases, the change occurred in a rather explicit and sudden manner, as the students were trying to justify their claims. The following interview excerpt captures the moment in which one of these two students seemed to undergo a mental model shift:

Like HBr . . . I know that’s very polarized because you know this is a lot more electronegative and it steals two electrons . . . and the hydrogen goes off and does it thing. So, that’s how I’m getting more acidic. I know acidic is proton donor? Giver, right? Yea, so acids give away hydrogen. Yea, Yea. (S10 justifying the answer to question #3)

In the case of S6, the shift from Mental Model B to Mental Model C was less definitive. During the explanation task, this student enriched his explanation by recognizing the role of resonance in the stabilization of chemical substances. This idea was then used to justify a change in previously predicted rankings for question #3, based on the relative stability of conjugate bases. However, this interviewee reverted to arguments that only considered composition and structural features of the acid in the rest of the justification tasks. Finally, for S4, the explanation task triggered the expression of Mental Model B through what seems an association of concepts ($pK_a \rightarrow \text{pH} \rightarrow \text{proton donor}$), but this model coexisted alongside, rather than replaced, the mental model expressed throughout the interview (Mental Model D).

The interview transcript of participant S4 was particularly interesting because it captured the struggle that many “multiple models” students had to reconcile assumptions from different models, given the diversity and constant misapplication of the ideas that they considered. For example, let us consider the following excerpt from the interview with S4 as he justifies his answer to question #7 (he had predicted $A < B < C$ in Figure 1 during the prediction task):

Int: . . . so, why did you choose A as being the least acidic?
S4: I think what I did was I picked A to be the least acidic because it has the most oxygens . . . And then, I guess I thought of stability and more delocalization of electrons on B. It would be a lot easier than on C. It would make B a little more stable than C . . . but I guess more evidence to back it up [his choice of A as least acidic] is that it has two oxygens which have three lone pairs on each of them. Making that least acidic, or actually. Yes, least acidic because it’s not giving away as many hydrogens which means C and B would have to be switched back around because B is more able to give up more hydrogens than C.

This interview excerpt is illustrative of how different assumptions about perceived relevant decision-making cues gained and lost strength as these students, particularly S4, reasoned through a given task. In this particular question, the assumption “stronger acids are better electron acceptors” only allowed S4 to justify his ranking for substance A. Thus, he relied on the assumptions “stronger acids are more unstable substances” and “charge delocalization stabilizes molecules” to justify his choice of C as the most acidic substance. However, the assumption “stronger acids are better hydrogen donors” was somehow triggered in his mind during the justification process which prompted him to change his ranking and propose B as the most acidic compound due to the presence of more hydrogen atoms in the molecule. Ultimately, the final ranking was based on the application of the assumptions underlying the two mental models that dominated this student’s thinking about acids during the interview (Mental Models D and B).

Discussion, Conclusions, and Implications

One of the central goals of our study was to characterize the mental models of acids and acid strength expressed by college organic chemistry students when engaged in different types of tasks. In particular, we wanted to uncover the underlying assumptions on which these mental models were based. Our study elicited four distinct mental models which guided study participants in making decisions and building explanations about relative acid strength (Table 1). Some of these expressed mental models are similar to those described by other authors. For example, Mental Model A resembles the “Character-Symbol Model” identified by Lin
and Chiu (2007) in their study involving ninth-grade students in Taiwan. On the other hand, the reasoning applied by organic chemistry graduate students in Bhattacharyya’s (2006) investigation shares many similarities with that of study participants who used Mental Model B to make ranking decisions in some cases but relied on Mental Model C for others. However, our work highlights the great diversity of mental representations that advanced students at the college level seem to have about acidic substances, and the sometimes contradictory assumptions that they make about the factors that influence their behavior.

Although some of the expressed mental models described in this work share many features with some of the scientific models of acids and acid strength developed by chemists (e.g., Mental Model B and Arrhenius model, Mental Model C and Brønsted–Lowry model, and Mental Model D and Lewis model), they can be better characterized as synthetic mental models (Vosniadou, 1994). Our students’ mental models were often hybrid models that combined assumptions from one or more scientific models with intuitive beliefs about factors that determine the properties of chemical substances. For example, the intuitive idea that the properties of chemical compounds are additive (Talanquer, 2006), and thus vary in proportion to the amounts of the components present in the system, was at the core of many of our students’ predictions, independently of whether they thought of acids as substances that lost protons or accepted lone electron pairs. As also suggested by recent research on college physics students’ mental models of heat conduction (Chiou & Anderson, 2010), our work indicates that hybrid models seem to be characteristic of the mental representations of advanced college students.

A second goal of our study was to analyze how task content and task type influenced the mental models used by students to generate answers. In this area our study revealed that (a) the presence of specific problem features or (b) changes in the nature of the task prompted some research participants to change their mental model or to add a different mental representation. In particular, we identified cases in which salient composition and structural features of the substances included in a given problem determined the type of mental model that was expressed, regardless of the type of task (e.g., prediction vs. explanation). However, there were also situations in which the work on the explanation and justification tasks prompted students to modify some beliefs or introduce new ideas to justify their decisions. These results underscore the dynamic nature of students’ mental models (Greca & Moreira, 2000) and the influence that context may have on the activation of relevant cognitive resources. In particular, our results support claims about the need for analyzing students’ reasoning in different contexts when making judgments about the coherence of their knowledge structures (diSessa, 2004).

Our analysis of how students used mental models to reason about acids and acid strength indicated that for many of our interviewees mental models served more as tools for heuristic decision-making based on intuitively appealing, but many times mistaken, concept associations rather than as cognitive tools to generate explanations. Particularly during the prediction tasks, many students relied strongly on intuitive beliefs and rules, such as the “More A–More B” heuristic (Stavy & Tirosh, 2000), and on specific prior knowledge about the substances of interest to generate their answers. Research participants tended to more thoughtfully engage in the process of manipulating mental models when their short-cut reasoning strategies failed. This was particularly characteristic of students that expressed Mental Models A, B, and D during the prediction task. In those particular cases where the switch from the prediction to the explanation or justification tasks triggered a change in expressed mental model, the new mental representation was often based on less intuitive and more scientific assumptions about the properties of acids. The explanations and justification tasks somehow prompted students to both enrich the nature of the cognitive resources used to deal with the problems at hand and apply more analytical versus heuristic ways of reasoning. The apparent triggering of different cognitive processes by different types of tasks has been observed by other researchers (Chiou & Brown, 2010; Schwartz & Black, 1996), and provides support to a dual-process model of reasoning (Evans, 2006). However, more experimental studies are needed to further explore this phenomenon.

The combination of intuitive beliefs and rules with assumptions from different chemical models of acids led many of our research participants to consider a multiplicity of irrelevant factors in making predictions and explaining trends in acid strength. This was particularly characteristic of students who expressed Mental Model B and multiple mental models. Interviewees who relied on Mental Model A or Mental Model C were more conservative in the number of cues used to make decisions. Students in these latter two groups represent opposite extremes with respect to the amount and accuracy of the prior knowledge elicited during the
Interview (Model A, lowest; Model C, highest), as well as in the level of “hybridization” of the mental models that they used. This suggests that average students in more advanced chemistry courses struggle to discriminate relevant factors in the prediction of chemical properties and to differentiate among different theoretical models used to describe and explain chemical behavior.

Although the organization of expressed mental models in Figure 1 may be suggestive of a learning progression (NRC, 2007), one should be careful with such an interpretation. Interviewees classified as expressing Mental Model A were certainly representative of students who seemed to hold very naïve and underdeveloped notions of acid and acid strength. On the other hand, students who expressed Mental Model C demonstrated the highest levels of understanding among the people in our sample. Thus, these two models may represent initial and more advanced stages in the progression of understanding of the targeted concepts at the college level. However, judgments about potential learning stages are more difficult to make in all of the other cases. Particularly because overall student performance depended not only on the nature of the mental model that was expressed, but also on factors such as relevant prior knowledge about specific substances (e.g., $pK_a$ values of known acids), ability to monitor one’s own reasoning (metacognition), level of local and global coherence in the application of ideas (diSessa, 2004), and reliance on heuristic versus analytical reasoning for decision making (Evans, 2006). Thus, within a single group listed in Table 1 we may have students with very different abilities to generate appropriate answers despite similarities in the general mental model of acid and acid strength that they used to guide their thinking.

Recognizing the limitations imposed by the small size of our student sample, our results are revealing of the complexities in the development of a meaningful understanding of more advanced ideas in the sciences. As college science students progress in their learning, they are exposed to a variety of models used by experts to describe, explain, and predict the properties and behavior of diverse systems. Most of these models are likely to be introduced without much discussion of their underlying assumptions, range of application, and intrinsic limitations (De Vos & Pilot, 2001; Furió-Más et al., 2005). Students can then be expected to generate hybrid concept associations or synthetic mental models that, despite general similarities like the ones outlined in our work, will be rather idiosyncratic and task-dependent. The design of effective instructional activities in this context becomes a real challenge, particularly if we take into account the large size of some science classes, such as organic chemistry, at many universities.

However, our results suggest that science instruction in advanced courses at the college level would benefit by a more careful analysis of the underlying assumptions and reasoning heuristics, both intuitive and instruction driven, that guide students’ construction of mental models in core topics and in different contexts. This knowledge would help instructors design learning opportunities that can better help students monitor their reasoning while engaged in specific tasks, by collectively analyzing the nature of the most common distracting factors and appealing reasoning heuristics for the less experienced thinkers. Our study also highlights the need to engage students in model-building and model-analysis activities that guide them in the construction of scientifically acceptable models and make them reflect on their range of application. Finally, the described effects of task content and task type on student reasoning indicate that properly diversifying and sequencing the nature of the academic tasks in which students are asked to participate (e.g., prediction vs. explanation) could better foster meaningful learning as different types of cognitive resources and ways of reasoning may be activated by different students, and thus shared, analyzed, and discussed.

References


Journal of Research in Science Teaching

