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Fan Yan & Vicente Talanquer

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Students' Ideas about How and Why Chemical Reactions Happen: Mapping the conceptual landscape

Fan Yan and Vicente Talanquer*
Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ, USA

Research in science education has revealed that many students struggle to understand chemical reactions. Improving teaching and learning about chemical processes demands that we develop a clearer understanding of student reasoning in this area and of how this reasoning evolves with training in the domain. Thus, we have carried out a qualitative study to explore students reasoning about chemical causality and mechanism. Study participants included individuals at different educational levels, from college to graduate school. We identified diverse conceptual modes expressed by students when engaged in the analysis of different types of reactions. Main findings indicate that student reasoning about chemical reactions is influenced by the nature of the process. More advanced students tended to express conceptual modes that were more normative and had more explanatory power, but major conceptual difficulties persisted in their reasoning. The results of our study are relevant to educators interested in conceptual development, learning progressions, and assessment.

Keywords: *Chemistry education; Conceptual development; Qualitative research*

Introduction

The description, explanation, and prediction of chemical reactions are fundamental goals of the chemical sciences. The mastery of ideas about chemical processes depends not only on students' conceptual understanding of a wide range of concepts, such as the particulate model of matter and chemical bonding, but also on students' ability to integrate these ideas and properly apply them in diverse contexts. Consequently, students often struggle to make sense of chemical phenomena (Barke, Hazari, & Yitbarek, 2009; Kind, 2004; Taber, 2002) and tend to rely on simple

*Corresponding author. Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ 85721, USA. Email: vicente@u.arizona.edu

heuristics and intuitive assumptions to guide their thinking (Talanquer, 2006). With training in the discipline, some students are able to develop normative understandings about chemical reactions, but many others are trapped in 'mixed' cognitive states where common sense ideas and pieces of disciplinary knowledge are combined in idiosyncratic ways to make sense of natural phenomena (Clark & Linn, 2003).

Recent efforts in science education highlight the importance of better characterizing how student understanding of core concepts progresses with studies in a discipline (National Research Council [NRC], 2011). These characterizations are not easy to build as they depend on long-term longitudinal studies that are difficult to carry out. However, we can gain critical insights by performing cross-sectional studies involving students at different educational levels, mapping common reasoning patterns at each level, and comparing them across groups. In this study, we followed such approach, seeking to map common ways of reasoning expressed by undergraduate and graduate students when thinking about how and why chemical reactions happen. We were particularly interested in exploring how the type of chemical reaction under analysis (combination, decomposition, and displacement) may influence student reasoning. This qualitative research study is part of a larger project focused on the characterization of changes in students' chemical thinking with training in the domain (Sevian & Talanquer, 2014; Weinrich & Talanquer, 2015).

Students' Ideas about Chemical Reactions

A variety of research studies have investigated students' ideas about chemical reactions (Barke et al., 2009; Kind, 2004; Taber, 2002). Several of these investigations have explored whether students recognize chemical change (Abraham, Williamson, & Westbrook, 1994; Calik & Ayas, 2005; Tsaparlis, 2003), and their findings reveal that pupils struggle to understand matter transformations. Many of these difficulties seem to stem from an underdeveloped concept of substance (Johnson, 2000, 2002; Ngai, Sevian, & Talanquer, 2014; Rahayu & Tytler, 1999; Stavridou & Solomonidou, 1989, 1998). Students often think that substances can change their properties but maintain their identity (De Vos & Verdonk, 1987), or talk about properties as materials that can be transferred from one substance to another (Sanmartí, Izquierdo, & Watson, 1995).

A significant number of studies have sought to characterize secondary school students' ideas about what happens to matter during a chemical process (Andersson, 1986, 1990; Boo & Watson, 2001; Prieto, Watson, & Dillon, 1992; Watson, Prieto, & Dillon, 1997). Results from these studies reveal that most students do not explain chemical reactions in terms of chemical interactions among submicroscopic particles. Rather, they tend to rely on surface macroscopic features of reactants and products to explain or predict the outcomes of chemical reactions (Ahtee & Varjola, 1998; Hesse & Anderson, 1992; Talanquer, 2008).

Many students have difficulties understanding why and how reactions happen. They often fail to differentiate between thermodynamic and kinetic factors influencing chemical processes (Boo, 1998; Thomas & Schwenz, 1998), and refer to chemical processes as driven by agents acting asymmetrically (e.g. active versus passive) in a system (Hatzinikita, Koulaidis, & Hatzinikitas, 2005; Taber & García-Franco, 2010; Talanquer, 2006). It is also common for students to attribute intentionality to chemical entities (e.g. electrons, atoms, and molecules) and assume that chemical processes take place to satisfy the needs or wants of these components (Taber, 2013; Talanquer, 2013).

Many educational research studies on chemical change have focused on the analysis of learners' alternative conceptions about different types of reactions. In particular, a variety of authors have investigated students' ideas about combustion reactions (Méheut, Saltiel, & Tiberghien, 1985; Prieto et al., 1992; Watson et al., 1997), acid–base reactions (Cros et al., 1986; Demerouti, Kousathana, & Tsaparlis, 2004; Nakhleh, 1994), and redox processes (Garnett & Treagust, 1992; Sanger & Greenbowe, 1997). These studies reveal the wide range of topic-specific difficulties associated with understanding the types of chemical interactions that occur under different conditions.

Theoretical Framework

Research findings in cognitive psychology suggest that human reasoning involves the dynamic interaction of a variety of cognitive elements (conceptual epistemological, ontological, and affective) that guide, but also constrain the explanations, predictions, and decisions that people make (Chi, 2008; diSessa, 1993; Vosniadou, 2014). Some of these cognitive resources function as heuristic rules for decision-making, while others resemble implicit assumptions about the properties and behaviors of entities and processes in our world (Talanquer, 2006). The nature of these cognitive elements, as well as their level of integration depends on personal characteristics and experiences. Their activation in a particular situation depends on contextual cues and loses or gains strength depending on perceptions of success in completing various tasks (Brown, 2014; Brown & Hammer, 2008).

Different authors have proposed that there is heterogeneity in the way people think and talk about concepts in different contexts (Gupta, Hammer, & Redish, 2010; Mortimer & El-Hani, 2014). For example, a person who feels cold may think of 'heat' as a material entity that can be contained in a room by closing the windows, and later conceptualize 'heat' as a process when engaged in an academic discussion on properties of materials. Personal experiences and sociocultural background affect how people learn and understand concepts, shaping the cognitive elements that are developed, their associations, and the contextual cues that trigger them. We may expect individuals with shared backgrounds to exhibit a similar profile of modes of thinking for a specific concept. However, the conditions, frequency, and consistency with which each of those modes of thinking will be deployed may strongly depend on personal characteristics (Mortimer & El-Hani, 2014).

Research on students' ideas about chemical reactions suggests that students actually have different ways of thinking and talking about chemical changes (Solsona, Izquierdo, & De Jong, 2003). For example, they may talk of some processes as driven by the intrinsic goals of an agent (e.g. atoms want to react to get an octet of valence electrons), while talking about other reactions as the result of random collisions between components (Talanquer, 2013; Weinrich & Talanquer, 2015). The identification and characterization of these different 'conceptual modes', the conditions under which they tend to manifest, as well as the analysis of their prevalence among different populations of students, may help us leverage student thinking and design learning opportunities that better scaffold the development of meaningful understandings.

Goals and Research Questions

The central goal of this study was to map and characterize common ways of reasoning (conceptual modes) about different types of chemical reactions (combination, decomposition, and displacement) expressed by students with different levels of training in chemistry. In particular, our study was guided by the following research questions:

- What are common reasoning patterns in students' explanations about *how* chemical reactions happen (*chemical mechanism*)?
- What are common reasoning patterns in students' explanations about *why* chemical reactions happen (*chemical causality*)?
- How do these conceptual modes vary depending on the type of reaction under analysis and on students' level of training in the domain?

Methodology

Research Context and Participants

This study was conducted in a research-intensive public university in the USA. At the time of data collection, the institution had close to forty thousand students (52.1% female, 47.9% male; 55.5% Caucasian, 19.6% Hispanic, 22% other minorities, and 2% unknown). The participants of this study were undergraduate and graduate students enrolled in different courses offered by the Department of Chemistry and Biochemistry at this institution. The undergraduate participants were registered in either second-semester general chemistry (a first-year course) or second-semester organic chemistry (a second-year course). The graduate participants were either first-year graduate students or Ph.D. candidates in the department. The undergraduate participants were recruited through an open announcement during a lecture session of the class and follow-up email invitations. The graduate participants were recruited via email invitations. All students consented to participate in the study without receiving any form of reward. A total of 65 volunteers participated, including 22 second-semester general chemistry students (G), 16 second-semester organic chemistry students (O), 13 first-year graduate students (F), and 14 advanced Ph.D. candidates (A).

Data Collection

We used semi-structured interviews as the main data collection tool to probe students' reasoning. The interview protocol included five common chemical reactions of various types: two combination reactions, two decomposition reactions, and one double displacement reaction (precipitation reaction). The selected reactions are listed in Table 1. Each of these processes was purposely chosen to investigate the influence of different explicit and implicit features of chemical representations on student reasoning, such as different types of states of matter of reactants and products, types of chemical substances, nature of chemical bonds, and types of reaction drivers (i.e. energetic versus entropic factors).

All interviews were conducted by the first author of this paper. During the interviews, each of the five reactions was shown on a different slide that included symbolic and particulate representations of reactants and products. Upon presentation of a slide, participants were instructed to think aloud as they answered questions about why and how each particular reaction happened. Paper and pencil were available for those who wanted to build personal representations of chemical structures or processes. The individual interviews lasted between 30 and 45 min and were audio-recorded and later transcribed. Participants' drawings were collected, scanned, and integrated with the corresponding transcriptions to better understand participants' explanations.

Data Analysis

Individual interview transcripts were analyzed following an interactive, constant-comparison approach (Charmaz, 2006). The first author of this paper analyzed all transcripts while the second author separately analyzed over 20% of them. The two researchers met on a regular basis to compare and discuss their individual analyses. During these meetings, the coding scheme was refined and all differences in code assignments were resolved by mutual agreement. These differences were mostly associated with initial divergences in how each researcher interpreted some codes that were resolved through discussion. Differences also occurred when students' expressed ideas that were difficult to understand. Consider, for example, the following excerpt: 'OK, so right here this double bond, neither one of those oxygens wants it. So I think the atom would start to shift around and replacing itself, so that it can change.'

Table 1. Chemical reactions included in the interview protocol

Reaction type	Chemical equation
Combination	$HCl(g) + NH_3(g) \rightarrow NH_4Cl(s)$
	$2\ Cu(s) + O_2(g) \rightarrow 2\ CuO(s)$
Decomposition	$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$
	$H_2CO_3(aq) \rightarrow CO_2(g) + H_2O(l)$
Double displacement	$AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$

In this case, it was not clear to which entities the student was referring or the nature of the mechanism she was invoking. In such circumstances, the two authors re-analyzed the whole transcript together and either agreed on a common interpretation based on the available data or eliminated the passage from the coding record. Less than 5% of all coded statements were discarded using this procedure.

Transcripts were first coded using an open-coding process to characterize students' ideas about the nature and properties of chemical substances and processes. Students' conceptions about how and why chemical reactions occur were highlighted and analyzed. Several categories of codes emerged from this work. These main categories were treated as potential dimensions in the characterization of student reasoning about causality and mechanism. These dimensions were refined and re-conceptualized as the data analysis process continued. Our work led us to identify six major dimensions in the characterization of students' ideas about the mechanism and causality of chemical reactions. We developed three dimensions to describe students' ideas about chemical mechanism (*how reactions start, how reactions proceed,* and *when reactions stop*), and another three to describe students' ideas about chemical causality (*why reactions happen, what drives reactions,* and *what determines reaction extent*). The boundaries between these two sets of categories are not sharply defined, since how things happen and why things happen are often related to each other. For example, some study participants claimed that chemical reactions occurred because of the attraction of particles of different types (why it happened) that led these particles to combine with one another (how it happened). In such cases, student reasoning about what drove the reaction and how it proceeded was strongly interconnected. In other cases, the relationship was much weaker as when students claimed that a reaction happened through the breaking and formation of chemical bonds (how it happened) and stated that the process was driven by a tendency of the particles to become more stable (why it happened). In general, the selected dimensions of analysis allowed us to highlight major differences in the ways of thinking about different types of chemical reactions among our study participants.

During our analysis, major ways of talking and thinking about a system or phenomenon were identified as different 'conceptual modes.' For example, in the dimension 'how reactions start', several students assumed that the more reactive reactant started a reaction by attacking other reactants. We categorized these types of explanations as belonging to the conceptual mode 'the more reactive reactant begins the process'. However, other students assumed that the reaction started by adding heat. This way of thinking was associated with the conceptual mode 'external agents initiate the process'.

Different conceptual modes in each dimension of analysis were constantly compared, refined, and then organized in increasing levels of explanatory power. Level of explanatory power was assigned by the researchers based on judgments of the extent to which a given conceptual mode could help propose generalizable mechanisms to describe, explain, and predict chemical phenomena. These judgments were informed by our own professional knowledge and by existing research on students' causal reasoning (Grotzer, 2003; Hatzinikita et al., 2005). The prevalence of a given conceptual mode in students' explanations was quantified by counting the number of reactions per individual interview in which such a conceptual mode manifested. A description of the nature and prevalence of the conceptual modes expressed by our study participants is presented in the following section.

Major Findings

Our analysis focused on the identification of students' ideas about how chemical reactions happen (chemical mechanism) and why they happen (chemical causality). In particular, we identified different ways of reasoning along the following dimensions:

- *Mechanism*: 1. How reactions start, 2. How reactions proceed, and 3. When reactions stop.
- *Causality*: 1. Why reactions happen, 2. What drives reactions, and 3. What determines reaction extent.

A summary of the conceptual modes that emerged from our analysis is depicted in Figure 1 organized in order of increasing explanatory power. All representations have

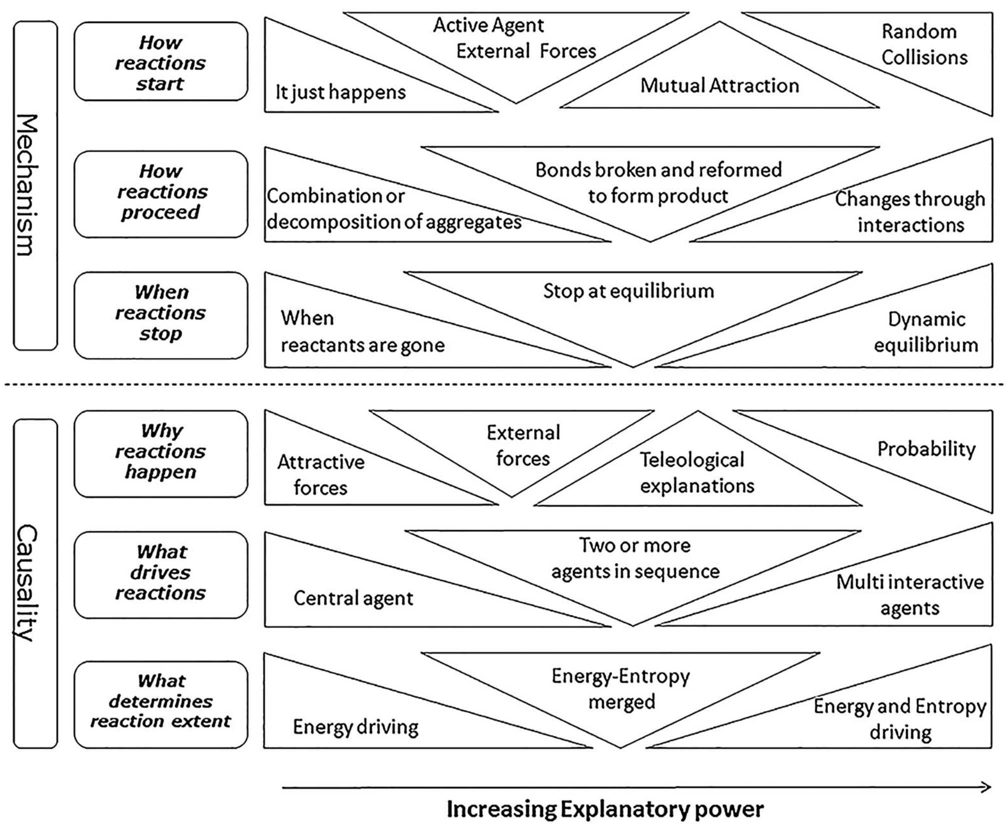


Figure 1. Common conceptual modes reflecting increasing level of explanatory power in each dimension of analysis

limitations and we do not intend to suggest that conceptual understanding progresses linearly through the different conceptual modes listed from left to right in this figure. Rather, Figure 1 should be interpreted as a map of common ways of thinking about different aspects of chemical reactions, representing diverse levels of sophistication in reasoning about mechanism and causality of chemical reactions. Major characteristics of these different conceptual modes are summarized in the following paragraphs.

Mechanism: How do the Reactions Happen?

We identified three major dimensions in the analysis of students' understanding of chemical mechanism related to *how reactions start*, *how reactions proceed*, and *when reactions stop*.

Dimension 1: How reactions start. During the interviews, many study participants discussed how they thought different reactions started. As summarized in Table 2, students' explanations within this dimension were classified into five different conceptual modes listed in order of increasing explanatory power as judged by the researchers. The table includes interview excerpts representative of each major conceptual mode.

The manifestation of the different conceptual modes listed in Table 2 depended on both the students' level of training in chemistry and the type of reaction under analysis. Figure 2(a) shows the percentage of instances in which each conceptual mode was detected in the explanations generated by different groups of students. In general, graduate students expressed conceptual modes with greater explanatory power (i.e. D1M4 and D1M5) than undergraduate students, but assumptions about the existence of an active initiator of chemical reactions (conceptual modes D1M2 and D1M3) were prevalent across all groups. Figure 2(b) depicts the distribution of conceptual modes for different types of chemical reactions. As this figure shows, students in our sample were more inclined to invoke the existence of an active internal initiator (conceptual mode D1M2) when analyzing combination reactions, but were more likely to claim that external forces initiated the process (conceptual mode D1M3) when thinking of decomposition reactions. Explanations associated with the double displacement reaction included a wider distribution of conceptual modes.

Some study participants expressed rather intuitive ideas about what initiates chemical reactions. They considered that chemical reactions just happened either spontaneously or by mixing substances (conceptual mode D1M1). When expressing this conceptual mode, students tended to focus on macroscopic events (e.g. decomposition or mixing of substances), without any reference to interactions or processes at the submicroscopic level. As shown in Figure 2(b), more students expressed this conceptual mode for the double displacement reaction than for the combination reactions and the decomposition reactions. No significant differences were observed in the frequency with which groups of students with different training in chemistry expressed this type of reasoning (Figure 2(a)).

Table 2. Conceptual modes for the dimension 'how reactions start' and representative interview excerpts

Conceptual modes		Interview excerpts
D1M1	It just happens	***G16:*** *Well, this, kind of looks like decomposition. So they, the original molecule came apart and then it would rearrange itself to make the products.*
D1M2	The more reactive reactant begins the process	***O3:*** *Because it's the strong acid, it's more reactive. It's more likely to completely dissociate and contribute to actually anything happening as opposed to the weak base, which is more likely just kind of sitting there until prompted.* ***F6:*** *I think the weak base is the one that's supposed to start the reaction. Because normally the nucleophilic groups are the one that attacks the electrophilic ones.*
D1M3	External forces initiate the reaction by breaking chemical bonds	***A6:*** *You need energy in the system to break the bond. And this HCl of course has bond energy. So if you could overcome bond energy, you might be able to break it to H and Cl.* ***G19:*** *So it has to be certain energy given to form the products. So it probably starts by having some sort of energy source, like a spark, or heat or something.*
D1M4	Reaction starts by attraction between particles	***F1:*** *And then as soon as they encounter each other, so it will be like two magnets, you can't really say one initiates more than the other, you know.* ***F7:*** *Initially it's going to begin with internal hydrogen bonding. And this lone pair is going to grab that hydrogen.*
D1M5	The reaction results from the random collisions or vibrations of particles	***F4:*** *I don't think either. They are both going to be moving at certain speeds. So you need both of them to pound in each other at the same time. In that case, it's not necessary initiation.* ***F11:*** *I would consider vibration would go like that. I would consider that it starts with combination with asymmetric vibration like that. So they go like that.*

Some study participants assumed that chemical reactions were started by an active agent acting on one or more passive components (D1M2). This way of thinking was more prevalent in the analysis of combination reactions, where a significant number of students at all educational levels considered that the strong acid or the oxygen gas were the active initiators of the processes (Figure 2). Students who expressed this conceptual mode often invoked intuitive attributes of agents (e.g. strength and ability to move) to justify their reasoning. More advanced students tended to refer to chemical properties (e.g. nucleophilicity) to justify the existence of a more active component (Table 2). In the case of the displacement reaction, where a more reactive reactant cannot be easily identified, students made different types of claims about the active agent, such as selecting the less stable reactant, the bigger ion, or the more

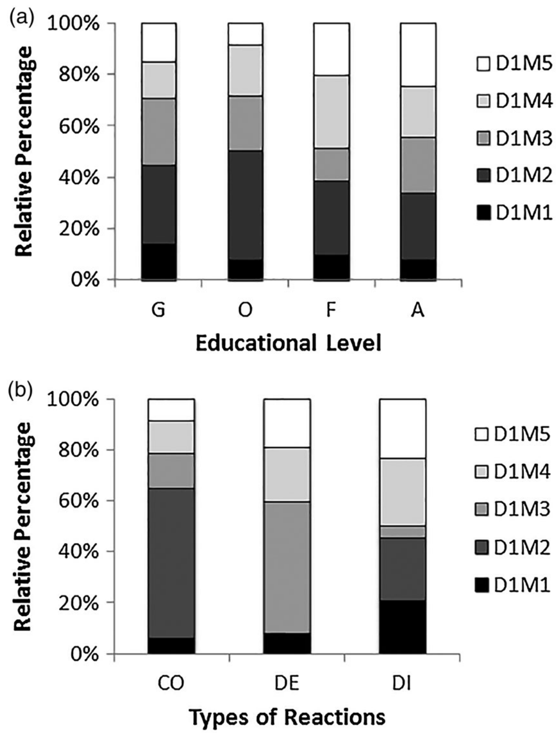


Figure 2. Relative percentage of study participants who expressed a given conceptual mode in the dimension 'how reactions start' per (a) educational level (G-General Chemistry, O-Organic Chemistry, F- First Year Graduate, A- Advanced Graduate), and (b) type of reaction (CO- Combination, DE-Decomposition, DI- Displacement)

electronegative species. Given that decomposition reactions involved a single reactant, conceptual mode D1M2 did not manifest in any of the students' explanations.

Students who expressed conceptual mode D1M3 assumed that external agents of forces, such as energy, heat, or a catalyst started chemical reactions mostly by causing bonds to break. This was the dominant way of reasoning expressed by students when thinking about decomposition reactions, but only a few students expressed it when considering combination reactions and double displacement reactions. Most students within this mode assumed that external drivers, such as heat, were needed to break reactants apart. Some students also assumed that external energy was needed to bring reactants together or sustain the reaction. In general, undergraduate students were more inclined than graduate students in our sample to think that the decomposition of a substance was driven by the action of external agents.

There were participants who assumed that chemical reactions started due to attractive forces between particles (D1M4). For reactions involving more than one reactant, these students considered that both reactants played an active role in the process. For decomposition reactions, students who expressed this conceptual mode assumed that the processes started with the attraction between parts within a single reactant. No significant differences were observed in the expression of this conceptual mode by students from different groups (Figure 2(a)). A larger proportion of students expressed this conceptual mode for the double displacement reaction than when thinking about combination reactions (Figure 2(b)).

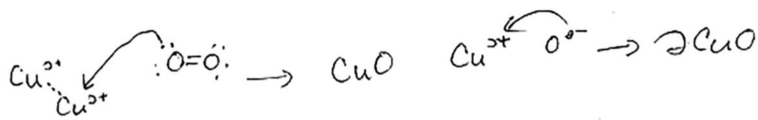
Students who expressed conceptual mode D1M5 described chemical reactions as resulting from random collisions between interacting particles. Chemical reactions happened when molecules of both reactants collided with each other with enough kinetic energy, or when molecular vibrations were strong enough to break chemical bonds. Students who expressed this conceptual mode built similar explanations for combination reactions and the double displacement reaction (Table 2). For decomposition reactions, students who expressed this conceptual mode often assumed that the processes started by internal atomic movements. More graduate than undergraduate students expressed this conceptual mode (Figure 2(a)). As was the case for conceptual mode D1M4, students were more likely to express this conceptual mode when thinking about displacement reactions and decomposition reactions than when reasoning about combination reactions (Figure 2(b)).

Dimension 2: How reactions proceed. This dimension characterized students' explanations about how the particles of reactants interacted with each other to produce the products. Three major conceptual modes, listed in Table 3 together with representative interview excerpt, were elicited from the analysis of students' explanations. The prevalence of these conceptual modes in the explanations of different groups of students and for different types of reactions is represented in Figure 3(a) and 3(b), respectively. In this case, study participants with more training in chemistry expressed conceptual modes with more explanatory power than the more novice students. This is particularly evident in the case of conceptual mode D2M3. In general, students generated more sophisticated explanations for the double displacement reaction than for other types of processes.

Students who expressed conceptual mode D2M1 assumed that chemical reactions resulted from the mere combination or decomposition of different pieces or components. These study participants could not provide details about reaction mechanism and seemed confused about how atoms were bonded to each other. When thinking about combination reactions, many of these students assumed that reactants just combined to form the products. Most students who expressed this conceptual mode referred to attractive forces due to the presence of opposite net charges or partial charges between components. In the case of decomposition reactions, students who expressed this conceptual mode often assumed that the reactant would break apart into pieces under the action of external agents, such as heat or catalysts. In general, when students expressed this conceptual mode they referred to submicroscopic particles as simple aggregates of parts that combined or separated to form different products (Table 3). This way of reasoning was dominant among general chemistry students, but rather marginal among other groups of study participants (Figure 3(a)).

Many of the students in our sample seemed to have a clear sense of how atoms were bonded in reactants and products, and assumed that these bonds broke and formed

Table 3. Conceptual modes for the dimension ‘how reactions proceed’ and representative interview excerpts

Conceptual modes		Interview excerpts
D2M1	Reactions are simple combination or decomposition of difference pieces	***G4:*** *Um, when you add heat, enough energy is released to actually break the bonds between the* $CaCO_3$ *molecules, and then will break apart and form* CO_2 *and CaO.*
D2M2	Chemical bonds are broken and formed to form targeted products	**O15:** *Copper two plus, and you would have a bond. I think oxygen would come in again to destroy the bond of copper. So you are left with CuO. And then you are also left with some copper two plus and oxygen two minus as a result of that. But then they react. And then you are left with more copper oxide, I think.* 
D2M3	Chemical bonds are broken and formed during chemical reactions due to particular chemical interactions	**F4:** *Once it runs into it, there has to be very quick exchange of hydrogen to the ammonium, which would be more ionized. Then you can start having everything go forward. I think that’s how it works You just have to get the HCl run into the ammonium, transfer the hydrogen, and then they are ionic and they should pair up, in order to pair up the electron cloud. It’s because they become too heavy to remain gaseous.*

during chemical reactions. However, they often had problems differentiating between different types of chemical bonds, treating covalent bonds as ionic bonds and vice versa, and thus misapplying chemical concepts and ideas in building explanations (conceptual mode D2M2). These study participants proposed mechanisms for chemical reactions in very idiosyncratic ways, referring to interactions and events that led to the formation of the targeted products but usually based on ad hoc transformations (Table 3). This conceptual mode was most prevalent among organic chemistry students in our sample, and manifested more commonly when thinking about combination and decomposition reactions (see Figure 3(a) and (b)).

Students with more advanced training in chemistry often were able to provide normative explanations about how particles of reactants interact, as well as about how chemical bonds break and form as a result of chemical interactions (conceptual mode D2M3). Proposed reaction mechanisms were built as sequences of events determined by the molecular composition and structure of interacting species, with good understanding of the different types of interactions that occurred depending on the nature of the reactants. As shown in Figure 3(b), a larger fraction of our study

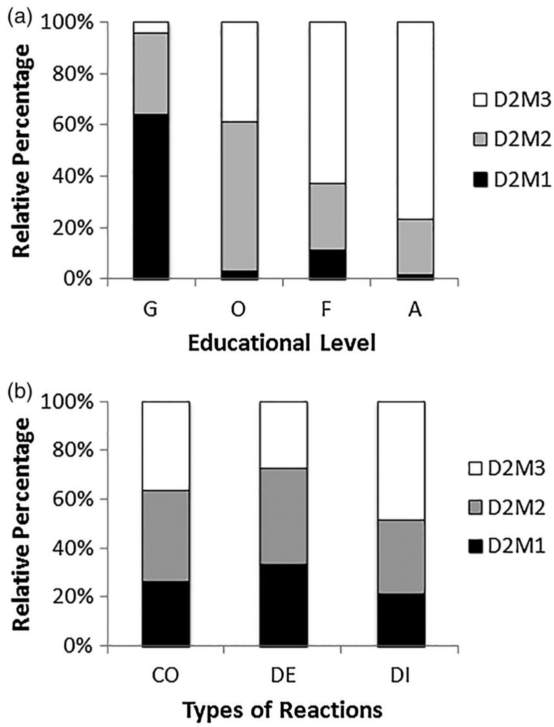


Figure 3. Relative percentage of study participants who expressed a given conceptual mode in the dimension 'how reactions proceed' per (a) educational level, and (b) type of reaction

participants applied this type of reasoning during the analysis of the displacement reaction than in their explanations of combination and decomposition reactions.

Dimension 3: When reactions stop. This dimension characterizes students' understanding of what happens in a chemical system when no more changes are detected. As summarized in Table 4, students' explanations along this dimension were classified into three major conceptual modes that manifested in the explanations of students with different levels of chemistry training (Figure 4(a)) for all types of reactions (Figure 4 (b)). In general, conceptual mode D3M1 was the most prevalent across groups of students and types of reactions.

Students who expressed conceptual mode D3M1 assumed that chemical reactions would go to completion and would literally stop when all the reactants or the limiting reagents were consumed. No significant difference was observed in the expression of this conceptual mode across different types of reactions. Interview excerpts illustrating different students' ideas about when the different reactions stop are included in Table 4. Most study participants assumed that there was a reactant that acted as the limiting reagent and when this substance was completely consumed, the reaction stopped. A few of students who expressed conceptual mode D3M1 mentioned chemical equilibrium, but considered that the reactions under analysis would not reach

Table 4. Conceptual modes for the dimension 'when reactions stop' and representative interview excerpts

Conceptual modes		Interview excerpts
D3M1	The reaction stops when the reactants are gone	***A10:*** *If something runs out, let's say if oxygen runs out, then you can go, um, the reaction will stop.* ***A14:*** *I think it's probably just block the oxygen getting into it. So once it's done oxidizing the surface, it will stop.* ***O1****: I don't think it's in equilibrium. So I think everything would probably go to the product side. So it would stop when all the products are gained.*
D3M2	The reaction stops at equilibrium	***O14:*** *I think it would stop when it reaches equilibrium, but I would guess again in the media that's ionized, it would get more towards the products than towards the reactants.* ***A3:*** *I am not sure about the equilibrium constant for this one, but I am assuming if it's not sealed container, the* CO_2 *can just escape. So you will always form the products until all your reactants are consumed. Then it will stop. But if it's in a sealed container, it will stop at equilibrium.*
D3M3	Dynamic equilibrium is assumed. The reaction never stops	***O12:*** *The percentage between the reactants and products would stay the same. That's what I consider as 'stopping'. But in reality, they are always going to be going on.* ***F7:*** *It's just you get equal amount of change from calcium carbonate to calcium oxide as calcium oxide to calcium carbonate. The reaction continues. It's just the net reaction doesn't continue.*

equilibrium because chemical equilibrium only applied to certain types of processes. As shown in Figure 4(a), this conceptual mode was dominant across different groups of students.

Some study participants assumed that the analyzed chemical reaction reached equilibrium, but the process stopped at that point (conceptual mode D3M2). Students who expressed this conceptual mode often assumed that chemical reaction favored the formation of products and that no more changes occurred once the system reached equilibrium. In some cases, study participants recognized that system conditions would affect the extent of the reaction, but considered that the reaction would stop when equilibrium was reached (Table 4). As shown in Figure 4(b), more students expressed this conceptual mode when analyzing decomposition reactions than other types of processes. The formation of a gas in these processes led several students to consider equilibrium ideas if the reaction were carried out in closed systems. Only a few students in our sample expressed conceptual mode D3M3, recognizing the existence of competing chemical processes at equilibrium (Table 4).

In general, the nature of the chemical reactions had a strong influence on students' assumptions about when and how chemical processes would 'stop.' Only 40% of our participants expressed the same conceptual mode when thinking about all three types

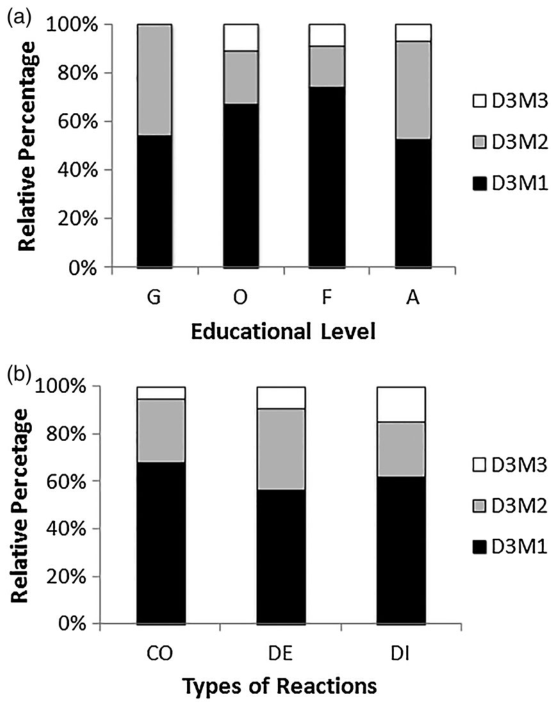


Figure 4. Relative percentage of study participants who expressed a given conceptual mode in the dimension 'when reactions stop' per (a) educational level, and (b) type of reaction

of processes. Students in our sample were more likely to assume that combination reactions and double displacement reaction would go to completion, while decomposition reactions involving gaseous products were thought to reach equilibrium in closed systems. The presence of particular states of matter, such as gases, substances, such as carbonic acid, or conditions, such as aqueous solutions, influenced students' ideas about the extent of the process, with more students entertaining ideas about chemical equilibrium in those circumstances.

Causality: Why do the Reactions Happen?

We identified three major dimensions in the analysis of students' understanding of chemical causality related to *why reactions happen*, *what drives reactions*, and *what determines reaction extent*. Some of the conceptual modes identified in these dimensions overlap with those associated with chemical mechanism as ideas about why reactions happen influence reasoning about how these processes occur, and vice versa.

Dimension 4: Why reactions happen. Analysis of students' ideas about what causes chemical reactions allowed us to characterize the five different conceptual modes listed in Table 5. Making judgments about the level of explanatory power of several

Table 5. Conceptual modes for the dimension 'why reactions happen' and representative interview excerpts

Conceptual modes		Interview excerpts
D4M1	Reaction happens because of attractive forces	***A10:*** *Okay, so I would think it in terms of interactions. So what we have here is silver interacting with water and nitrate interacting with water, and also sodium interacting with water and chloride interacting with water. Interactions between silver and chloride are stronger than interactions between silver and water, silver and nitrate. Therefore, silver and chloride will come together and precipitate.*
D4M2	Reaction happens because of external forces	***G12:*** *Because of the input of the energy, because this probably would not happen spontaneously, I wouldn't just say calcium carbonate magically dissociates into these two products. So, um, the reaction happens because of the outside energy put in.*
D4M3	Reaction happens because the products are more stable or at lower energy states	***O5:*** *I guess because it wants to form … in nature, things want to have lowest energy state as possible, and bonds, and orientation, and things are arranged all to contribute energy of molecules and space and space like physical space. You know, if this is formed, the reactants are less energy than the, no, no, the products are less energy than the reactants. That's why it happens because doing all this will produce a less energy state molecule than the previous things before.*
D4M4	Reaction happens because particles of reactants break up with external forces, and then rearrange to form more stable products	***G11:*** *What happens is, since you increase the energy, it breaks the bonds. The molecules are, or the atoms are all separated. And since, when they are all separated, they are not stable. So the attractions between them force them to come together to more stable forms, CO_2 and H_2O.*
D4M5	Reactions happen because of random interactions of chemical particles	***F6:*** *Again molecules keep hitting on each other … And maybe these collisions become more energetically as time progresses or temperature increases… I mean it's like you have two small particles that keep vibrating on each other. And at one point, one of them becomes gaseous… Maybe they form back calcium carbonate. It's just that they don't see themselves as much as they were, because basically one is gaseous anyhow, and another is a solid. So they don't see themselves as much as they used to. So the reaction still happens, but maybe at very small chances.*

of these ways of thinking is quite difficult. Consequently, the labels associated with each conceptual mode are mostly intended to differentiate them rather than to rank them. Conceptual modes D4M1 and D4M2 involve linear causal explanations in which a single event or process is seen as the cause of change. Conceptual modes D4M3 and D4M4 rely on teleological thinking in which processes are talked about as the result of the needs or wants of different components. Conceptual mode D4M5 implies a more probabilistic causal view of chemical reactions. The prevalence of these different conceptual modes in the explanations of different groups of students and for different types of reactions is represented in Figures 5(a) and (b), respectively.

Students who expressed conceptual mode D4M1 assumed that reactions simply happened due to attractions between or within the reactants. This conceptual mode was expressed most commonly when thinking about displacement reactions and to a lesser extent when talking about combination reactions (Figure 5(b)). For this latter type of reactions, students usually assumed that the two reactants had opposite characteristics, such as electric charge or acid–base character, that brought them together. In the case of displacement reactions, students often assumed that the

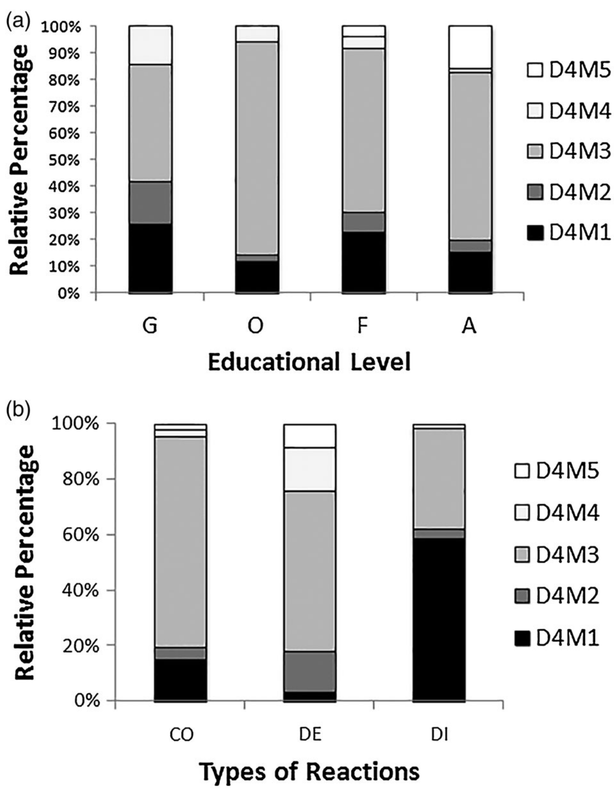


Figure 5. Relative percentage of study participants who expressed a given conceptual mode in the dimension 'why reactions happen' per (a) educational level, and (b) type of reaction

process happened because interactions between some ions (e.g. silver and chloride ions) were stronger than interactions between other ions.

Some students considered that chemical reactions occurred due to the action of external agents or forces that caused substances to break apart. This conceptual mode (D4M2) was mostly expressed when thinking about decomposition reactions. Students who expressed this way of reasoning tended to think of chemical reactions as processes that required external energy input to separate particles and facilitate their rearrangement. In general, conceptual modes D4M1 and D4M2 were expressed by students at all educational levels but were not dominant in most students' explanations.

Conceptual mode D4M3 was the most commonly expressed by our study participants. This type of reasoning was based on teleological arguments to explain why reactions happened. In particular, students invoked a 'purpose' for the change, which often was the need or want of an entity or system to adopt a more stable or a lower energy state. Students who expressed this conceptual mode often use anthropomorphic language to describe the goals and actions of chemical species. Although one can suspect that not all students believed that atoms, molecules, or ions had actual needs or desires, many of the study participants who expressed this conceptual mode were unable to generate causal explanations when prompted. Teleological arguments were built not only in terms of attaining energetic stability, but also based on the system's desire to become more random or increase its entropy.

Conceptual mode D4M4 can be conceived as a hybrid of conceptual modes D4M2 and D4M3, and mostly manifested in the analysis of decomposition reactions. In this case, students assumed that reactions happened because reactants were broken apart by external forces, and the resulting pieces rearranged to produce more stable product. In most cases, students invoked energetic stability considerations but some of them generated entropic arguments (i.e. the system wants to become more disordered).

Very few students in our sample expressed conceptual mode D4M5 based on the assumption that chemical reactions happened because of random collisions between particles, and the probability of forming products was higher than that of forming reactants. Study participants who manifested this type of reasoning often build initial teleological explanations, but were able to provide causal accounts when prompted. As shown in Figure 5(a) and (b), most students who expressed this conceptual mode were advanced graduate students and they did it more frequently when analyzing decomposition reactions.

Dimension 5: What drives reactions. This dimension allowed us to characterize students' ideas about the agents that drive chemical reactions. We used the term 'agent' to refer to either components of a chemical system or properties of such components assumed to influence reaction extent and rate. As shown in Table 6, three major conceptual modes were identified along this dimension. These conceptual modes differ in the number of agents that were invoked and in the relationships assumed among them. Figure 6(a) and (b) depict the prevalence of these conceptual modes in the explanations generated by students at different educational levels and for different types of reactions.

Table 6. Conceptual modes for the dimension 'what drives reactions' and representative interview excerpts

Conceptual modes		Interview excerpts
D5M1	Reactions are driven by one central agent	***G15:*** *I am guessing that heat would be a factor and breaking it up. Because the bonds probably not held together incredibly tightly, so what happens is heat, or some kind of light would heat it and it would decompose into calcium oxide and* CO_2.
D5M2	Reactions are driven by two or more agents acting in sequence	***O3:*** *I believe it would probably start with some introduction of energy, probably heat. And that energy allows the bond to break, and then separate into the calcium oxide and carbon dioxide … That is allowed to be broken. And then there is positive charge on calcium. It's seeking out electrons. All these oxygens, I believe it would have a partial negative charge. So it's able to form a bond with one of the oxygens.*
D5M3	Reactions are driven by multiple interactive agents	**A8:** *So basically when they collide with each other, you have the transfer of proton from the HCl to* NH_3 *to form* NH_4*. And then because you have electrostatic interaction between the Cl minus and the* NH_4 *plus, so basically you form a unit of a crystal… And if this collides with this, and they just transfer that proton. Then you have Cl minus and* NH_4 *plus. And because they have opposite charges, then they would attach each other to form the units… The reactants have higher energy than the products. So basically to lower the energy, they become more stable.* ***G1:*** *Well going from something that's a solid to something that's a salt and a gas, so that implies that it's entropically unfavored. And then you are also going from more complex molecule to a less complex molecule, which doesn't apply there is energetically either unfavored or only slightly favored… And it only happens at high temperature because that's only, that's the only point where that the molecules are going fast and they are starting to get each other… Well, when* $CaCO_3$ *are going fast enough, the molecules start hitting each other more rapidly. When they hit each other harder, um, it has a higher chance to break the bonds and reach the transition state. If the transition state goes to product, then what will happen is it doesn't keep the bond and the bond is broken, and displaced, and it's replaced, or just let it low how it is, and that's how you get the CaO or* CO_2.

In general, conceptual mode D5M1 was dominant in the explanations of undergraduate students while conceptual mode D5M3 gained prevalence with increasing training. Along this dimension, study participants were able to generate more sophisticated explanations in the analysis of displacement reactions.

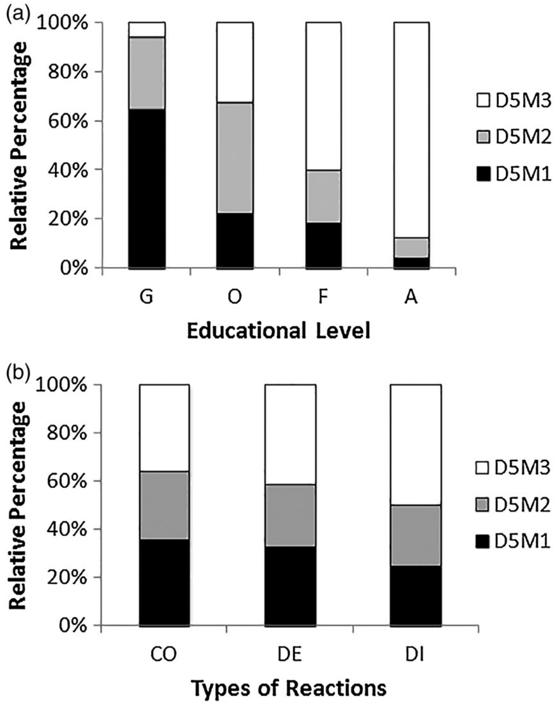


Figure 6. Relative percentage of study participants who expressed a given conceptual mode in the dimension 'what drives reactions' per (a) educational level, and (b) type of reaction

Students who expressed conceptual mode D5M1 often identified a single central agent that triggered or caused the reaction to happen. Common agents included chemical species (atoms, molecules, ions, electrons) with a partial or net electric charge that exerted attractive forces on other entities. These types of explanations were particularly common in the analysis of combination and displacement reaction. In the case of decomposition reactions, students were more likely to invoke heat or a catalyst as central agents. As shown in Figure 5(b), conceptual mode D5M1 was common among general chemistry students, but its frequency significantly decreased among other groups of students.

Some students built explanations that tended to invoke two major agents as drivers of chemical processes, describing their actions in sequential ways (conceptual mode D5M2). For example, some students assumed that external forces could break chemical bonds and generate charged species that then rearranged according to their interactions. Other students referred to collisions between particles as responsible of bond breaking and to attractions between charged species as responsible for bond formation. In general, these students tended to think of one agent as causing bond breaking and another agent causing bond formation. This conceptual mode was most commonly observed in the explanations built by organic chemistry students (Figure 6(a)).

Students who expressed conceptual model D5M3 were able to identify multiple agents as drivers of chemical reactions. However, there were major variations in the extent to which different study participants considered interactions or relationships between these agents. For example, several students referred to different factors, such as electronegativity, polarity, and bond strength in their analysis of chemical reactivity, and identified important relationships between them. However, they built explanations that focused on the properties of single particles without taking into consideration the effect of multi-particle distribution and interactions (e.g. entropic considerations). Only a small fraction of students in our sample, mostly at the graduate level, built more comprehensive explanations that took into account thermodynamic (energetic and entropic factors) and kinetic factors.

Dimension 6. What determines reaction extent. The dimension 'what determines reaction extent' allowed us to characterize whether students could recognize how energetic and entropic factors affect reaction extent. Analysis of students' explanations along this dimension led us to elicit the three major conceptual modes listed in Table 7. The prevalence of these different conceptual modes in explanations of students at different educational levels is represented in Figure 7, where we can see that the conceptual mode D6M1 was dominant across most groups, except the advanced graduate students. In fact, this was the only conceptual mode observed in students' explanations

Table 7. Conceptual modes for the dimension 'what determines reaction extent' and representative interview excerpts

Conceptual modes		Interview excerpts
D6M1	Energetic factors determine reaction extent	***G13:*** *So like the other one we are going to a lower energy state, and now this one is like a higher energy state. And so with that higher energy, um, maybe, since we are putting energy into the system, this is obviously higher energy, and so perhaps in order to go to, like the low energy state, they would have to split in order to like, I guess, even out the energy, like their peer to high energy state, and then they split, and that's like, once the energy is split, then it's kind of relax again.*
D6M2	Merged ideas about the effect of energetic and entropic factors on reaction extent	***F4****: You know, the only thing come into my mind is that it's completely circular just saying entropic effects. You know, the universe always want to go to the least high-energy system, so, yeah, just entropic effects. You want to go to a lower energy system. A lower energy system is always preferred by the way the universe works, described by the laws of thermodynamics, I guess.*
D6M3	Both energetic and entropic factors determine reaction extent	***A12:*** *So you have two salts and a gas. First of all, you entropy is going to go up, which is a good thing. So this ΔG is equal to ΔH minus $T\Delta S$. This is bond-making, which is favorable processes. And this is entropy increasing for favorable processes again.*

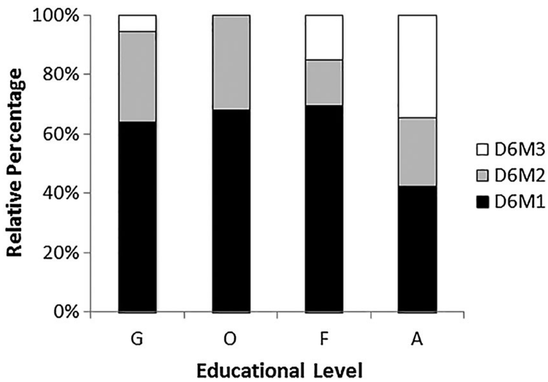


Figure 7. Relative percentage of study participants who expressed a given conceptual mode in the dimension 'what determines reaction extent' per educational level

of combination and displacement reactions. For decomposition reactions, D6M1 manifested in 61% of all instances, while conceptual modes D6M2 and D6M3 corresponded to 26% and 13%, respectively.

Students who expressed conceptual mode D6M1 only focused on energetic factors when discussing the extent of chemical reactions, ignoring entropic considerations. Although the directionality of the two decomposition reactions included in our research instrument is mostly determined by entropic effects, many students built explanations centered on energetic issues. Many of these students judged that chemical reactions would take particles to lower energy states, without considering that the processes might be endothermic and actually result in higher potential energy products. This 'bias' toward energy-focused explanations was common across all groups of students and all types of reactions.

Some students considered both energetic and entropic factors as relevant in analyzing why the reactions happened. However, they often exhibited misunderstandings about the influence of different factors or failed to conceptually differentiate energy from entropy (conceptual mode D6M2). Students who expressed this type of reasoning recognized that entropic factors had to be taken into account to make judgments about the directionality of the chemical processes, but often assumed that 'more disorder' meant 'lower energy,' reducing entropic arguments to energetic considerations. Only a small fraction of our study participants, mostly advanced graduate students, properly analyzed energetic and entropic factors to judge reaction directionality and extent (conceptual mode D6M3). In general, students were less able to consider and justify why an increase of entropy would drive a reaction forward than they could explain why a decrease in the energy of the system would favor the formation of products.

Discussion and Implications

The central goal of this study was to uncover students' conceptual modes about chemical mechanism and causality when analyzing different types of chemical reactions. The major conceptual modes elicited through our investigation are summarized in Figure 1 where they have been organized along the core dimensions of analysis that emerged from our study. These different conceptual modes represent common ways of thinking and talking about different aspects of chemical reactions. Although their prevalence in students' talk depended on the level of training in chemistry and on the type of reaction under analysis, some of them were dominant in the explanations generated by most students in our sample.

Our results revealed the common use of agentive arguments to explain chemical processes by students at all educational levels. Most students tended to identify an active species (e.g. the more reactive reactant) or external forces (e.g. heat, catalyst) as the agent that initiated chemical reactions, and often talked about chemical processes as driven by the needs or wants of these agents to achieve a more stable state (teleological arguments). These results are aligned with previous findings by different researchers (Hatzinikita et al., 2005; Taber, 2013; Taber & García-Franco, 2010; Talanquer, 2006). Many students failed or struggled to explain why the more stable states would be formed based on normative chemical ideas, and when they did, they mostly built energetic arguments neglecting entropic considerations. Similarly, most study participants did not express a dynamic view of chemical reactions in which final states involve chemical equilibrium between competing processes.

Major differences between groups of students at different educational levels were observed in their explanations of how a reaction proceeds and what agents affect the process. As revealed by previous studies (Andersson, 1990; Hesse & Anderson, 1992), the more novice learners tended to think of chemicals as physical aggregates that simply combine or break apart during chemical transformations, without a clear idea of what happens at the molecular level. More advanced undergraduate students tended to conceptualize chemical processes as involving bond breaking and bond formation, but often proposed idiosyncratic mechanisms to generate the desired product (Bhattacharyya & Bodner, 2005). The ability to build causal mechanistic explanations based on multiple interactions between various agents was mostly constrained to the advanced graduate students in our sample.

The type of chemical reaction under analysis had a significant influence in the conceptual modes expressed by students. Different explicit features of the represented chemical reactions (e.g. number of reactants involved, state of matter of reactants and products, known properties of the substances involved) seemed to trigger different assumptions about chemical mechanism and chemical causality. For example, most students talked about internal active agents that acted to achieve desirable states when building explanations for combination reactions, while they mostly referred to the action of external forces to justify decomposition reactions. In general, students built more causal mechanistic explanations when thinking about double displacement reactions where the actual mechanism is easier to infer from the composition and structure of reactants and products. Similarly, students' consideration of chemical equilibrium was highly sensitive to explicit features in the representation of chemical reactions (e.g. aqueous solutions, formation of gases).

The generalizability of our findings is certainly limited by the qualitative nature of our research involving a small number of volunteer students at each educational level and a few types of chemical reactions. In this regard, we plan to use the results of our study to develop a questionnaire that can provide quantitative information about the prevalence of the different reasoning patterns elicited by this investigation. Our interpretation of students' conceptual modes is also affected by our own personal beliefs about how students think and learn, and about the nature of chemistry knowledge. However, our results represent a snapshot of student reasoning about chemical reactions with important implications for chemistry teaching and learning.

The meaningful understanding of how and why chemical reactions happen demands the development and integration of a wide variety of concepts and ideas, from chemical bonding to chemical kinetics and thermodynamics. Our results suggest that the development of such understanding may take considerable training, may not occur at the same pace along different dimensions, and may be highly sensitive to contextual issues such as the types of reactions under analysis. Previous work suggests that it also may be highly dependent on the type of task (e.g. evaluating a reaction's feasibility versus proposing a reaction to generate a desired product) (Weinrich & Talanquer, 2015). These considerations pose a major challenge to current curricular, instructional, and assessment practices, particularly at the post-secondary level.

The organization of chemistry curricula tends to be rather segmented. At the course level, content is often organized around topics (e.g. stoichiometry, atomic structure, carbonyl chemistry) making it difficult for the students to integrate ideas and recognize common ways of thinking across different contexts. At the program level, courses are traditionally divided into traditional areas (e.g. general, organic, and analytical chemistry) where concepts and ideas are often presented using different disciplinary frameworks that fail to make explicit common ways of thinking. A curricular organization around major chemistry crosscutting concepts, such as structure–property relationships and chemical mechanism, could help better support progressive knowledge integration (Sevian & Talanquer, 2014).

From an instructional perspective, chemistry courses are often taught using an explanation–application format in which information is first delivered by the instructor and then applied to solve specific problems. Seldom are students engaged in exploratory activities involving data analysis, using and building models to explain trends in the data, generating arguments from evidence, and creating mechanistic explanations of the systems under consideration (NRC, 2011). Our results suggest that many students would benefit from more active engagement in the construction and evaluation of explanations using different conceptual modes, comparing and contrasting their explanatory power in explicit ways. Different conceptual modes may be useful in different contexts and students need opportunities to identify and reflect on the productivity of their application.

Our findings also indicate that we should carefully reflect on the types of reasoning that different contexts demand to more carefully scaffold learning tasks. For example, students in our sample seemed to more easily understand the mechanism of double displacement reactions but struggled to make sense of decomposition reactions. An educational approach focused on the development of mechanistic reasoning would require a more careful consideration of the sequence of systems and processes with which students are confronted to challenge and advance their thinking.

Finally, our results also have major implications for the assessment of student learning. One of the major insights of our study is that the conceptual mode expressed by students was highly sensitive to the nature of the reactions under consideration. That poses a major challenge to the assessment of student understanding, as student performance may strongly vary from problem to problem. Additionally, it is unlikely that the types of closed-answer problems used in traditional assessments will elicit the actual conceptual mode applied by a student to generate or identify an answer. Diversification of assessment methods, and of the context of their application, may help generate more valid and reliable data about student understanding (Holme et al., 2010).

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