EXPLORING THE PROGRESSION IN STUDENTS' UNDERSTANDING OF CHEMICAL REACTIONS ACROSS DIFFERENT GRADE LEVELS

by

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ABSTRACT

EXPLORING THE PROGRESSION IN STUDENTS' UNDERSTANDING OF CHEMICAL REACTIONS ACROSS DIFFERENT GRADE LEVELS

This study aimed to map students' conceptual progression of how and why chemical reactions happen across different grade levels. This study also investigated how students' patterns of understanding change with respect to the type of chemical reaction under analysis. A total of 77 students participated in the study from different grade levels: Grade 12 students in high school level (n=20), Undergraduate 1 chemistry students (n=20), Undergraduate 4 chemistry students (n=20), and Graduate chemistry students (n=17). Grounded theory was utilized as the research methodology and semistructured individual interviews were conducted with the participants. Semistructured interview protocol included four types of chemical reactions (i.e., single displacement, double displacement, decomposition, and combination) based on particle arrangements. Through constant comparative analysis of the data, dimensions and conceptual modes were identified and conceptual modes were sequenced based on increasing sophistication. Data analysis showed that students' understanding of how and why chemical reactions happen depended on the grade level and the reaction type under analysis. The findings showed that the participants' understanding demonstrated progression regarding how chemical reactions proceed and chemical causality as the grade level increased. The participants mostly struggled while explaining the agents, processes, energetic, and entropic factors affecting chemical reactions. Therefore, the expression of the conceptual modes regarding the dimensions of what causes chemical reactions and what drives chemical reactions was lower when compared with the other dimensions. The findings of the study seemed to provide insights into designing curriculum, developing assessment tools and instructional practices.

ÖZET

FARKLI SINIF SEVİYELERİNDEKİ ÖĞRENCİLERİN KİMYASAL TEPKİMELERE İLİŞKİN KAVRAMSAL GELİŞİMLERİNİN İNCELENMESİ

Bu çalışmanın amacı farklı yaş gruplarındaki öğrencilerin kimyasal tepkimelerin nasıl ve neden gerçekleştiğine dair kavramsal gelişimlerinin incelenmesidir. Çalışmada ayrıca, öğrencilerin kimyasal tepkimelerin neden ve nasıl gerçekleştiğine ilişkin kavramsal anlamalarının farklı tepkime türleri için ne gibi değişiklikler gösterdiği araştırılmıştır. Çalışmaya dört farklı sınıf seviyesinden toplam 77 öğrenci katılmıştır. Bu çalışmaya 20 lise 12. sınıf öğrencisi, kimya bölümünden 20 lisans 1. sınıf öğrencisi, 20 lisans 4. sınıf öğrencisi ve 17 lisansüstü öğrencisi katılmıştır. Araştırma metodu olarak temellendirilmiş kuram kullanılmış olup, katılımcılarla yarı-yapılandırılmış birebir görüşmeler yapılmıştır. Yarı-yapılandırılmış görüşmeler taneciklerin dizilimine göre sınıflandırılmış dört farklı tepkime türü içermektedir ve bu tepkime türleri şunlardan oluşmaktadır: tekli yer değiştirme, ikili yer değiştirme, ayrışma ve birleşme. Elde edilen verilerin sürekli karşılaştırmalı analiz tekniğiyle incelenmesi sonucunda temalar ve kategoriler belirlenip, kategoriler kendi içlerinde kapsayıcılık seviyelerine göre sıralanmıştır. Yürütülen veri analizi ortaya koymuştur ki; öğrencilerin kimyasal tepkimelerin neden ve nasıl gerçekleştiğine dair algıları sınıf seviyesi ve tepkime türüne göre değişkenlik göstermektedir. Ayrıca, ilerleyen sınıf seviyesi ile birlikte öğrencilerin kimyasal tepkimelerin sürecine ve sebeplerine ilişkin kavramsal anlamalarında önemli gelişme olduğu gözlemlenmiştir. Katılımcıların en çok kimyasal süreçleri etkileyen etkileşimler, enerji ve entropi gibi faktörleri açıklarken zorlandıkları, ve ilgili kategorilerin frekanslarının diğer kategorilere kıyasla düşük olduğu görülmüştür. Çalışmanın bulguları, müfredat hazırlama, ölçme-değerlendirme araçları oluşturma ve öğretim yöntemleri geliştirme gibi araştırma alanlarında fayda sağlayabilecek çıkarımlar ortaya koymuştur.

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LIST OF SYMBOLS

f	Frequency
M	Mean
n	Number of participants in a group of the sample
Ν	Number of participants in the sample
T	Temperature
ΔG	Change in Gibbs energy
ΔH	Change in enthalpy
ΔS	Change in entropy
ΔS_{surr}	Entropy change in surroundings
ΔS_{sys} ΔS_{univ}	Entropy change in system
ΔS_{univ}	Entropy change in universe

LIST OF ACRONYMS/ABBREVIATIONS

AAAS	American Association for the Advancement of Science
G12Pn	nth participant in Grade 12 group
GRPn	nth participant in Graduate group
MoNE	Ministry of National Education
NRC	National Research Council
UG1Pn	nth participant in Undergraduate 1 group
UG4Pn	nth participant in Undergraduate 4 group

1. INTRODUCTION

Understanding, describing, and predicting chemical reactions are essential to make sense of physical sciences (i.e., physics and chemistry), as well as other domains of science. Demonstrating sophisticated understanding of chemical reactions depends on mastery of various concepts such as, particulate nature of matter, intermolecular and intra-molecular forces, particle interactions, energy, and laws of thermodynamics. More importantly, students' ability to integrate these concepts and adapt them to various contexts play a crucial role in deeper understanding of chemical reactions (Yan and Talanquer, 2015). Because of the content requirements and cognitive skills that students need to demonstrate, they have difficulties in making sense of chemical reactions (Talanquer, 2006). Thus, this study focuses on the reasoning patterns of students on chemical processes and builds a data informed learning progression that describes how their reasoning develops as they progress through chemistry education.

1.1. Chemical Reactions in Science Education Standards and National Curriculum

National Research Council (NRC, 2012) established that chemical reactions is one of the fundamental ideas in physical sciences (chemistry and physics) based on previous works for enhancing science education in the USA, such as *Benchmarks for Science Literacy* established by American Association for the Advancement of Science (AAAS, 2009). Systems and processes at any scale depend on physical and chemical sub-processes. Understanding such processes and natural phenomena requires comprehending particulate nature of matter, interactions among particles, and energy transfers (NRC, 2012). Therefore, it is essential to enhance students' understanding of cause and effect mechanisms in systems of any scale with an emphasis on physical and chemical processes. In order to present the significance of the study through the lenses of chemical reactions and related concepts, this section describes the accumulation of chemical reactions and concepts related with chemical reactions in the science education standards of the USA and in the science and chemistry curricula in Turkey. NRC considers chemical reactions among the component ideas of the disciplinary core idea of *Matter and Its Interactions*. Other component ideas are: *Structure and Properties of Matter* and *Nuclear Processes* (NRC, 2012). NRC strongly suggests creating learning environments for students to understand these ideas and their relations with one another. Furthermore, NRC proposes learning progressions for each of the component ideas which is in alignment with the ideas proposed by AAAS (AAAS, 2009). In the subsequent paragraphs, first, learning progressions regarding chemical reactions proposed by NRC (2012) are described in the USA context. Then, accumulation of the concepts regarding chemical reactions in the context of Turkey is presented to establish similarities and differences between these contexts.

By the end of Grade 2, students are expected to comprehend that heating and cooling substances may result in physical changes (i.e., phase changes) or chemical changes (e.g., burning, cooking), which are described as reversible and irreversible processes, respectively. By the end of Grade 5, students are supposed to realize that mixing substances together may cause formation of a new substance. This formation depends on temperature and the nature of the substances that are mixed together. It was also mentioned that total weight is conserved. By the end of Grade 8, students are introduced to the fact that some substances react together by the rearrangement of the particles that these substances are composed of. They are also expected to realize that the new substances formed as a result of such chemical reactions have different properties than the reactants. In addition, students are expected to understand that total number of particles and mass are conserved. At this stage, they are expected to be familiar with the fact that some reactions release energy, some of them absorb energy. Finally, by the end of Grade 12, students get familiar with collision theory, bond energies and dynamic nature of forward and reverse reactions. Thus, they are expected to connect these ideas and comprehend chemical reactions in terms of energy changes (whether energy is released or absorbed) as a result of particle collisions and rearrangements to form new substances, and changes in total bond energies. NRC suggests that, understanding rearrangement of the particles to form new molecules helps students to explain and predict chemical reactions.

In Turkey, there is a central science curriculum for Grades 3-8 (MoNE, 2013b). This science curriculum suggests that the main purpose of the science course is to enhance scientific literacy of the students with an emphasis of science, technology, society, environment, and basic domains in science; such as, biology, matter and changes in matter, physical phenomena, and the earth and the universe (MoNE, 2013b). Chemical reactions have a fundamental place under *matter and changes in matter* domain. In Grade 3, in addition to classifying matter based on hardness, color, texture, etc. by using five senses, students are expected to classify matter according to their physical states without mentioning their properties. In Grade 4, students are supposed to classify matter based on their physical states and give examples for each state. Additionally, they are expected to compare the properties of different states and design experiments related to phase changes upon heating and cooling. Finally, students are expected to classify everyday materials as pure and mixtures with an emphasis on differences between them. However, it was specified that particulate nature of matter is not mentioned at this stage. In Grade 5, states of matter and phase changes are introduced in a more detailed manner. In addition, effects of heating on matter are discussed in terms of expansion and contraction. Particulate nature of matter is introduced to the students in Grade 6, followed by physical and chemical change concepts with an emphasis on the differences between these changes. In Grade 7, students are supposed to be familiar with the concepts of atom, molecule, proton, neutron, and electron. They are expected to comprehend that the same or different kinds of atoms form molecules. They also classify substances as pure and mixtures, specifically, as element, compound, and mixtures. Grade 8 students are expected to explain the concept of chemical bond and classify them in terms of ionic and covalent characteristics. Finally, Grade 8 students are introduced to the chemical reactions and define chemical reactions in terms of bond breaking and bond formation with an emphasis on the conservation of mass. Concerning chemical reaction types, they are only introduced to the combustion and acid-base reactions (MoNE, 2013b). In high school (Grades 9-12), chemistry is started to be taught as a separate discipline and has a separate centralized core curriculum (MoNE, 2013a). Recently, Ministry of National Education established a new updated chemistry curriculum (MoNE, 2018). However,

during the data collection period (at the end of Spring 2017 term), the participants of this study were received their instruction based on the chemistry curriculum published in 2013 (MoNE, 2013a). Therefore, chemical reactions and related concepts in the Turkish context were described regarding the chemistry curriculum published in 2013 (MoNE, 2013a). Concept of chemical reactions has a fundamental place in the chemistry curriculum. Throughout the chemistry education, students are re-introduced to particulate nature of matter, electrostatic interactions among particles, and physical and chemical changes in a more detailed manner. In the subsequent years, they deal with different types of chemical reactions (e.g., combustion, acid-base, precipitation, and redox reactions) in addition to basic laws of thermodynamics and spontaneity of chemical reactions. Furthermore, they study chemical reactions in terms of molecular collisions, activation energy, chemical kinetics, reaction mechanisms, and chemical equilibrium (see Chapter 3.3) (MoNE, 2013a).

Considering the learning progressions that NRC proposed and the curricular progression described for Grades K-12 by the Ministry of National Education, students are supposed to explain, describe, and predict chemical reactions as dynamic processes in terms of energy related concepts and the dynamic process of the interactions among the particles of the reactants. As students progress through chemistry education over the years, they get familiar with the particulate nature of matter, intermolecular and intra-molecular attractions among the particles and their effects on the physical and chemical properties of the substances, and thermochemistry.

1.2. Rationale and Significance of the Study

1.2.1. Learning Progressions

Constructivist view of learning suggests that students actively build knowledge about natural phenomena, rather than receiving a transferred form of knowledge (Driver *et al.*, 1994). Students come to science classes with preexisting ideas about the natural phenomena, as a result of their physical and social interactions with their environments and instruction (Driver, 1989; Talanquer, 2006; Vosniadou, 2014). Research suggested that these ideas often differ from the scientifically accepted predictions, explanations, and practices which are to be introduced in the science classes (Barke *et al.*, 2009; Driver, 1989; Talanquer, 2006). These ideas affect students' learning and are found to be resistant to change (Driver, 1989). Therefore, identification of these ideas helps students build scientifically accepted understandings and is important to characterize the conceptions held by students in certain age groups to develop learning progressions (Adadan and Yavuzkaya, 2018; Talanquer, 2006).

Over the several years, researchers have been investigating the development in students' ideas in particular domains. Learning progressions help educators develop and connect standards/objectives, instructional strategies, and assessment tools (Duncan, 2009; Furtak, 2012; Furtak *et al.*, 2014; Songer *et al.*, 2009). Furtak (2012) stated that learning progressions, as a basis for curriculum, may also guide instructors and teachers in interpreting students' ideas of a particular scientific concept by shaping their instruction and assessment practices.

NRC (2007) defined learning progressions as "descriptions of the successively more sophisticated ways of thinking about a topic that can follow one another as children learn about and investigate a topic over a broad span of time" (p. 214). Songer et al. (2009) then suggested that in addition to sequencing topics of a particular content based on increasing levels of sophistication, learning progressions should also include increasing levels of sophistication in reasoning skills. It is argued that learning progressions place the scientific literacy at the core of the development of standards, instruction, and assessment tools (Duncan, 2009; Duncan et al., 2009). Therefore, big *core ideas* from a particular science discipline that are essential to promote scientific literacy are selected by the educators. However, this does not reveal students' path of learning as they progress through a science discipline. Learning progressions also encourage the organization of these ideas based on how students' thinking improves from naïve to sophisticated (Alonzo and Gotwals, 2012). This range of sophistication in students' understanding of a scientific content is described by synthesizing existing literature on a particular content under analysis or based on empirical research such as cross-sectional designs and longitudinal studies (Duncan, 2009). To be more specific, learning progressions are anchored by upper and lower ends. Upper end describes what students are supposed to know at the end of the progression. This anchor is based on the particular disciplinary content and the expectations of the society. Lower anchor is based on the knowledge of the learning progression developers about students' preexisting knowledge at the beginning of the progression. Yet, learning progressions also propose intermediate steps of understanding between upper and lower anchors (Plummer, 2014). These steps are determined by the literature analysis and empirical research (Duncan, 2009; Mohan *et al.*, 2009; NRC, 2007; Stevens *et al.*, 2010). Sequencing these steps also provides evidence for curriculum development while sequencing the standards (Fortus and Krajcik, 2012). Therefore, it is clear that there is a need for empirical research on students' thinking on a particular scientific content in order to inform the development of learning progressions.

1.2.2. Core Concepts in Chemistry

Current science education framework suggests that understanding science and engineering enhances scientific literacy in addition to helping future scientist and engineers since individuals need to make decisions related to everyday life, such as choosing containers for food or alternatives among various fuel types. Therefore, scientific literacy is essential for every individual, not just to the ones who pursue careers in science and engineering (NRC, 2011). In order to promote students' understanding in science and engineering, NRC (2011) suggests that students' understanding in crosscutting core concepts of science and engineering should be deepened. Through the K-12 education, students are expected to engage in scientific inquiry and engineering practices in order to pose answers to these issues.

In the context of chemistry education, there is a tendency to introduce various chemistry concepts in an isolated way. However, chemistry, as a scientific discipline, requires posing and answering authentic questions, such as how to synthesize a targeted product (for example, a surfactant), how to identify and store a pollutant. In order to address this authentic concerns of chemistry discipline, big core ideas and practices should be determined and integrated (Sevian and Talanquer, 2014). Smith *et al.* (2006)

suggested that these big ideas should have the following characteristics as they developed learning progressions on matter and atomic-molecular theory for particular big ideas:

- (i) Central to the discipline and have a broad explanatory power
- (ii) Contribute to the growth of the discipline and interconnect with the other fields
- (iii) Understood progressively in sophisticated ways
- (iv) Should form a foundation for the progressive learning

Research on learning progressions and students' alternative conceptions in chemistry usually focuses on mapping students' understanding of fundamental chemistry concepts, such as, chemical bonding. However, Sevian and Talanquer (2014) proposed another approach which emphasizes on tracking students' conceptual progression of *crosscutting disciplinary concepts* which are found to be fundamental for the basic practices of chemistry discipline, namely, investigation (understanding and predicting chemical properties), design (analyzing, synthesizing, and transforming matter for a particular purpose), and evaluation (evaluating the benefits and the costs of chemical practices). The crosscutting key concepts determined by Sevian and Talanquer (2014) are:

- *Chemical identity:* How chemical substances are identified
- *Structure-property relationships:* How properties of chemical substances are determined
- Chemical causality: Why chemical reactions happen
- Chemical mechanism: How chemical reactions happen
- Chemical control: How chemical reactions are controlled
- Benefits-costs-risks: How the effects of chemical transformations are determined

These crosscutting disciplinary concepts are considered to be fundamental in tracking students' understanding of fundamental chemistry concepts such as chemical bonding. The main purpose of this framework is to analyze how students use these fundamental chemistry concepts, like chemical bonding, while thinking about how chemical reactions happen (chemical mechanism). Sevian and Talanquer (2014) claimed that students' reasoning on these concepts gets sophisticated as they progress through chemistry education.

Among these crosscutting disciplinary concepts, this study focuses on *chemical mechanism* and *chemical causality*. More specifically, this contribution aims to identify and characterize how students' *conceptual modes* manifest themselves when analyzing different types of chemical reactions. This approach allows us to highlight conceptual progression of students from various educational backgrounds and from various chemistry education levels (i.e., grade levels). Investigating how students' conceptual modes regarding chemical processes evolve as they progress through chemistry education serves as a template. Furthermore, it enables educators to develop research based assessment tools, instruction techniques, and curricula, which promote students' understandings regarding these crosscutting disciplinary concepts.

1.3. Purpose of the Study

The main purpose of this study was to explore students' conceptual progression of how (chemical mechanism) and why (chemical causality) different chemical reactions (i.e., displacement, decomposition, and combination reactions) happen across different grade levels (i.e., Grade 12, Undergraduate 1, Undergraduate 4, and Graduate). In doing so, the study identified the patterns in students' understanding about how and why chemical reactions happen and organized them according to their levels of explanatory power. Consequently, the study explored how students' patterns of understanding about how and why chemical reactions happen change across different grade levels (i.e., different levels of chemistry education). Finally, the study also investigated how students' patterns of understanding change with respect to the type of chemical reaction under analysis.

1.4. Research Questions

In order to attain the goals stated in Section 1.3, following research questions guided this study:

- (i) How do students' conceptual modes related to chemical mechanism change across different grade levels?
- (ii) How do students' conceptual modes related to chemical causality change across different grade levels?
- (iii) How do students' conceptual modes related to chemical mechanism and chemical causality change with respect to the type of reaction under analysis?

1.5. Summary

This chapter started with emphasizing on the importance of chemical reactions among the core ideas as a fundamental basis for scientific literacy since it is connected with and form a foundation for understanding various ideas in chemistry, as a scientific discipline. Then, it was suggested that in order to develop a research informed curriculum, instruction and assessment practices, it is a necessity to investigate students' thinking on a particular scientific content and how their thinking evolves as they progress through chemistry education. Therefore, this study is based on two basic elements. First, as the scientific content, this study focuses on chemical reactions since it was established that chemical processes are among the big ideas to promote scientific literacy. Most of the research studies on students' conceptions in chemistry focuses on establishing students' understanding in fundamental concepts in chemistry, such as, chemical bonding. However, the framework used in this study suggests analyzing students' understanding of big ideas as lenses to see students' conceptions of the fundamental chemistry concepts, such as chemical bonding and particulate nature of matter. Second, it is essential to track how the understanding of the crosscutting disciplinary concepts evolve as students move through chemistry education in order to design and align curriculum, instruction, and assessment practices that revolve around the core ideas of chemistry to enhance scientific literacy.

Based on the two basic elements described above, this study aims to map students' conceptual progression on chemical mechanism and chemical causality as they progress through chemistry education. The following chapter describes the literature on students' understanding of chemical reactions with an emphasis on the constructivist view of learning. In Chapter 3, participants and the research methodology, which is a cross sectional design based on grounded theory on students' conceptual progression of chemical mechanism and chemical causality, is introduced. Chapter 4 describes the findings of the study and poses detailed answers for the research questions. Chapter 5 summarizes the findings and proposes implications for curriculum, instruction, assessment practices in addition to the implications for the future research.

2. LITERATURE REVIEW

2.1. Overview

The main purpose of this study was to investigate students' conceptual progression of how and why chemical reactions (displacement, decomposition, and combination reactions) happen across different grade levels (Grade 12, Undergraduate 1, Undergraduate 4, and Graduate). Specifically, the study aimed to identify students' reasoning patterns of about how and why chemical reactions happen and explore how students' patterns of understanding about how and why chemical reactions happen change across different grade levels (i.e., different levels of chemistry education). The study also aimed to investigate how students' understanding of why and how chemical reactions happen change with respect to the type of chemical reaction under analysis.

In order to address the purposes of this study, in the previous chapter, the research objectives were introduced as a need to explore students' understanding how and why chemical reactions happen and to create a research-based learning progression that depicts students' sophisticated manners of understanding of those two crosscutting disciplinary concepts of chemistry. This contribution may help researchers to develop aligned curriculum, instruction, and assessment tools that promote scientific literacy.

This chapter, first, describes constructivist view of learning, conceptual understanding and how learning progressions are related with constructivism and conceptual understanding frameworks. Then, it summarizes research studies on learning progressions in chemistry discipline. Finally, research studies on students' understanding of chemical reactions are described in detail. These studies cited in this chapter provide insight into what is known about students' understanding of chemical reactions and what remained unexplored.

2.2. Students' Conceptions and Learning Progressions

Research in science education and cognitive psychology shows that students come to science classes with preexisting knowledge about natural phenomena, because from early ages, they explore their surroundings by constant experimentations and social interactions and build concepts about various phenomena (Barke *et al.*, 2009; Duit and Treagust, 2003). These concepts are called *preconceptions* (Vosniadou, 2013). However, research on students' conceptions also show that these concepts that students build might differ from scientifically accepted ones and they are resistant to change (Driver, 1989; Reiner *et al.*, 2000; Taber, 2001; Treagust and Duit, 2008). Such conceptions are frequently called as alternative conceptions/presuppositions or synthetic models which can be held before and even after particular interventions to overcome them (Chi *et al.*, 2012; Vosniadou, 2013).

Students' preconceptions affect their interpretation of newly introduced phenomenon, and this affects the knowledge that they construct, their reasoning, and problem solving skills (NRC, 2000; Taber, 2003). This view of learning is based on constructivist view suggesting that students are active learners constructing their knowledge based on what they already know, their prior experiences, social interactions, attitudes, and beliefs (Barke et al., 2009; Driver, 1989; Driver and Leach, 1993; NRC, 2000; Taber, 2001; Taber, 2014). In other words, learning is an active process on which students have control (Clements and Battista, 1990; Driver, 1989). Conceptual understanding refers to constructing knowledge, using it in another contexts and problems, and connecting ideas (Stevens et al., 2010). On the other hand, when students come to classes with unorganized knowledge structures, they have difficulties in applying their knowledge to new problems and contexts. Additionally, it might be difficult for students to make sense of the presented ideas in the class because of their already existing ideas (Brown, 2014). Contrary to novice students, experts demonstrate well organized knowledge revolved around big ideas and core concepts in their disciplines (NRC, 2000; Stevens et al., 2010).

Researchers and teachers explore students' conceptions in order to diagnose their knowledge. By doing so, they determine appropriate intervention strategies and design curricula to promote their understanding. Driver (1989) claimed that even though such studies provide evidence for instruction and curriculum designs, they do not depict the dynamics of how students' conceptions change. Similarly, Wilson (2009) stated that a developmental perspective depicts how students' understanding of a particular concept progresses over time. Driver (1989) put an emphasis on the importance of tracking the patterns of change in students' conceptions (conceptual progression), because conceptual progression studies inform curriculum, assessment, and instructional strategies.

Driver's claims (1989) indicate that research on learning progressions is not a new idea. Educators and cognitive psychologists have been investigating the development in students' conceptions over several years in various disciplines (Duncan, 2009). In NRC's report (2007), it was mentioned that learning progressions align curriculum, instruction, and assessment. In contrast with the current standards, which include too many isolated concepts, NRC suggested organizing the standards and science curricula which are based on big ideas and crosscutting disciplinary concepts (NRC, 2007). According to NRC (2007), making such organization allows tracking the conceptual development that students are supposed to demonstrate. This understanding encourages considering students' already existing knowledge and their subsequent understandings (Duncan, 2009). It was stated that research informed assessment tools provide evidence for students' thinking about natural phenomena and the extent of their thinking. These assessment tools, therefore, help teachers to understand their students' thinking and align curriculum standards and students' experiences about natural phenomena (Smith et al., 2006). Learning progressions help connecting standards and students' thinking to develop assessment tools because standards mostly include only the statements of knowledge that students are expected to demonstrate, not the operational definitions of understanding. Lack of operational definitions in the standards creates a need for elaboration in order to develop assessment. Research on students' learning plays a complementary role for developing standards revolving around the big ideas of the domain under consideration which can provide basis for valid assessment tools (Smith et al., 2006).

Smith et al. (2006) defined learning progressions as "... descriptions of successively more sophisticated ways of reasoning within a content domain based on research syntheses and conceptual analyses." (p. 1). In their report, NRC (2007) elaborated this definition as "... descriptions of the successively more sophisticated ways of thinking about a topic that can follow one another as children learn about and investigate a topic over a broad span of time." (p. 214). As a contribution to these definitions, Songer et al. (2009) then suggested that in addition to sequencing topics of a particular content based on increasing levels of sophistication, learning progressions also include increasing levels of sophistication in reasoning skills. In addition to the content focus, learning progressions also put emphasis on inquiry skills, which are central to scientific literacy (Duncan, 2009). In order to promote scientific literacy and provide deeper content coverage, it was suggested that curricula and standards should limit the content and focus on crosscutting disciplinary concepts and core ideas (Bernholt and Sevian, 2018; NRC, 2011; Opitz et al., 2017). Therefore, current focus of science education is to explore students' understanding of crosscutting disciplinary concepts and core ideas across a time span (Bernholt and Sevian, 2018). Bernholt and Sevian (2018) suggested that there is a need for research on students' conceptual development across a time period and students' reasoning pathways that lead to intended learning outcomes.

Research studies on learning progressions in science have emerged in various types (Duncan, 2009). First, learning progressions are hypothetical which represent development of students' conceptions on core ideas or crosscutting concepts over time. These learning progressions are developed based on existing literature on the science concepts under consideration and the analysis of that science discipline (Duncan, 2009). For example, Smith *et al.* (2006) developed a hypothetical learning progression for K-8 level based on matter and atomic-molecular theory concepts. In this study, the authors determined the big ideas regarding matter and atomic-molecular theory and created a framework for assessment. Moreover, they elaborated the standards based on research on science education and developed assessment tasks based on the standards that they elaborated. A similar study was conducted by Duncan *et al.* (2009) on modern genetics for Grades 5-10. First, the authors determined the big ideas and the learning outcomes (i.e., knowledge and skills) regarding modern genetics by the end of education. Second,

the authors described the progression in students' learning as they progress through curriculum. Finally, assessment tools were determined based on the learning progression that the authors described. Stevens *et al.* (2010) developed a hypothetical learning progression on nature of matter for Grades 7-14 and proposed instructional strategies to facilitate students' construction of structured knowledge. Such studies aimed to provide insight into developing aligned curriculum/standards, instruction, and assessment tasks and items in order to promote students' understanding of core scientific concepts and enhance their scientific inquiry skills. Moreover, these studies provided basis for empirical research studies on learning progressions in science.

It was suggested that there is a need for empirical research studies in order to validate the hypothetical learning progressions (Duncan, 2009). These empirical studies are based on cross-sectional and longitudinal designs that track the development of students' conceptions of core ideas or crosscutting disciplinary concepts. This type of research does not involve instructional interventions. Rather, they depict the development of pathways in students' understanding of core ideas and crosscutting disciplinary concepts (Duncan, 2009). These empirical studies are mostly based on cross-sectional designs in which data are collected from various student groups (e.g., different grade levels) at a single point of time. Longitudinal designs, on the other hand, require a long period of time and are difficult to perform (Yan and Talanquer, 2015). These empirical studies usually involve both development and the empirical validation of the progressions (Mohan et al., 2009; Schwarz et al., 2009). Other studies, focus on students' conceptual progression on crosscutting disciplinary concepts and core ideas such as energy (Opitz et al., 2017). Opitz et al. (2017), for example, aimed to explore progression in middle school students' (Grades 6, 8, and 10) understanding of energy concept in physics, chemistry, and biology contexts. The researchers found that the students held single energy concept across physics, chemistry, and biology contexts. Results also showed that students' understanding of energy across different disciplinary contexts improved from Grade 6 to 10. In order to improve teaching and learning of energy concept across different disciplinary contexts, several instructional approaches were proposed such as relating energy concept across different disciplines.

Finally, some research on learning progressions involve sequentially designed instructional interventions and demonstrate students' potentials when they are scaffolded with a series of interventions. These intervention studies focus on learning contexts, curriculum, and assessment items and the relationship of these elements with students' complex thinking and reasoning skills (Cooper *et al.*, 2012; Plummer, 2014; Plummer and Krajcik, 2010; Plummer and Maynard, 2014; Songer *et al.*, 2009). These multi-step studies, first, design the learning progressions and instructional interventions and then track the progress in students' understanding with various methods, such as individual interviews and surveys (Cooper *et al.*, 2012; Plummer, 2014; Plummer and Krajcik, 2010; Plummer and Maynard, 2014; Songer *et al.*, 2009).

Given the research background on learning progressions in science, there are various methods of embedding learning progressions in science education to promote students' understanding of science and their scientific literacy. It was suggested that longitudinal studies, which integrate curriculum, instruction and assessment practices, are required to validate proposed learning progressions because under current instructional conditions, students' reasoning skills are not well developed (Duncan, 2009).

2.3. Learning Progressions in Chemistry

Currently, teaching approaches in chemistry seem to introduce chemistry concepts in a fragmented and isolated way (Sevian and Talanquer, 2014). However, this approach contradicts with current vision of science education, which intends to develop students' understanding of crosscutting disciplinary concepts and core ideas in the context of scientific inquiry over several years of science education (NRC, 2011). In order to enhance students' understanding of the crosscutting concepts and core ideas of a scientific discipline, learning tasks should engage students in scientific inquiry in which students learn to pose and answer authentic questions (NRC, 2011; Talanquer, 2016).

In order to engage students in authentic practices, it was suggested to integrate core ideas and practices within and across disciplines. Specifically, in chemistry, this pursuit involves studying chemical substances and explaining their properties and their interactions (Sevian and Talanquer, 2014). In the context of recent learning progressions that Sevian and Talanquer (2014) developed, they introduced the term *chemical* thinking as "... the development and application of chemical knowledge and practices with the main intent of analyzing, synthesizing and transforming matter for practical purposes." (p. 10). Core ideas related with analyzing (identifying, quantifying, and separating chemical substances), synthesizing (designing synthesis mechanisms for chemical substances), and transforming (control of chemical processes) matter are seen as fundamental for scientific literacy, because every individual, whether they are seeking career in science or not, has to make informed decisions concerning scientific issues (e.g., choosing an appropriate fuel and how to store food) in everyday life. With the hypothetical chemical thinking learning progressions, Sevian and Talanquer (2014) described the pathways that students progress through based on core practices of chemistry as they engage in chemical thinking (i.e., analyzing, synthesizing, and transforming matter) during chemistry education. These core practices are investigation (understanding and predicting chemical properties), design (analyzing, synthesizing, and transforming matter for a particular purpose), and evaluation (evaluating the benefits and the costs of chemical practices). Instead of the dominant approach which investigates students' understanding on certain chemistry concepts (e.g., chemical bonding, chemical kinetics, and energy), chemical thinking learning progressions focus on investigating the progression in students' understanding of crosscutting disciplinary concepts found to be fundamental in chemical thinking. Crosscutting disciplinary concepts determined by Sevian and Talanquer (2014) are:

- Chemical identity: How chemical substances are identified
- *Structure-property relationships:* How properties of chemical substances are determined
- Chemical causality: Why chemical reactions happen
- Chemical mechanism: How chemical reactions happen
- Chemical control: How chemical reactions are controlled
- Benefits-costs-risks: How the effects of chemical transformations are determined

These crosscutting disciplinary concepts provide basis for investigating students' understanding of fundamental chemistry concepts. For example, students' understanding of chemical bonding can be investigated while they are engaged in a core chemistry practice based on determining the properties of chemical substances. However, it is important to note that if these concepts are introduced by transferring basic knowledge without addressing the authentic issues that these crosscutting concepts refer to, students' learning will not be more than knowledge acquisition as it is done by traditional instructional and assessment practices (Talanquer, 2016).

The foci of this study were the two crosscutting disciplinary concepts, namely, *chemical mechanism* and *chemical causality* that are judged to be critical in mastering core practices of chemistry discipline. Regarding the crosscutting concepts that Sevian and Talanquer (2014) proposed, some empirical studies and critical analyses of the literature and the discipline were performed. These studies will be discussed in the subsequent paragraphs.

Chemical identity, as a crosscutting disciplinary concept, deals with one of the core practices of chemistry which is "how chemical substances are identified" and involves knowledge and skills regarding identifying chemical substances (Ngai et al., 2014; Talanquer, 2016). It is considered as one of the crosscutting disciplinary concepts that scientifically literate individuals need to be familiar with in order to identify chemical substances (Ngai et al., 2014). Ngai et al. (2014) proposed a hypothetical learning progression on chemical identity based on the existing literature on students' alternative conceptions and analysis of chemistry discipline. They analyzed the papers investigating how students identify and define different types of matter and what features they pay attention to while classifying matter. Ngai et al. (2014) investigated the change in assumptions that the students hold as they progress through chemistry education. They found that students' understanding of chemical identity progress in time but this progress is not linear. For example, they reported that novice students' reasoning regarding chemical identity is affected by appearance, usage, and history which are similar to the properties considered while identifying objects. With the introduction of chemistry concepts in submicroscopic level in high school years, students' views seemed

to shift from macro to submicroscopic, but even in graduate level, criteria that students used for categorization of matter were not stable and depend on the type of substance under analysis and the representation of the substances in the classification tasks. These results indicate that even though students' understanding of chemical identity gets sophisticated gradually as they progress through chemistry education, there is still a need for scaffolding students in developing their understanding. Therefore, it was suggested that students should be scaffolded by engaging them in investigating, designing, and evaluating tasks in contextual learning environments instead of simply covering fundamental chemistry concepts such as chemical bonding (Ngai *et al.*, 2014).

The concept involving structure-property relationships focuses on the fact that physical and chemical properties of matter are based on submicroscopic structure and interactions among particles. This concept plays a key role in determining, analyzing, synthesizing, and evaluating chemical substances and controlling chemical processes (Talanquer, 2016, 2018). In a recent paper, Talanquer (2018), performed a critical analysis of the literature to portrait students' conceptual progression on structure-property relationships. Critical analysis of the literature showed that students' reasoning about structure-property relationships seem to develop as they progress through education. However, it seemed that students' reasoning is affected by a set of implicit schemes that are slightly affected by instruction. Basically, students associate chemical composition of the substances and the properties as they ignore structural properties of the materials. Novice students tend to think that properties of materials depend on the natural characteristics. As they progress through chemistry education, they start to consider particulate nature of matter and think that the properties of materials depend on the type and number of atoms composing that material. More advanced students, on the other hand, consider dynamic interactions of the particles of chemical substances. Even though students' understanding gets sophisticated over the years, it depends on the system under analysis and students' familiarity and prior experiences with the system. Talanquer (2018) suggested that targeted instructional interventions should be developed to facilitate students' reasoning about structure-property relationships.

The concept involving benefits-costs-risks is related to the economic, environmental, and social consequences of analyzing, synthesizing, and transforming matter (Sevian and Talanquer, 2014; Szteinberg et al., 2014; Talanquer, 2016). In order to investigate students' progression in reasoning about making choice among different types of fuel, researchers conducted individual interviews with middle school (senior), high school (senior), and first year undergraduate students about deciding on the best fuel to use for a GoKart (Banks et al., 2015). Results revealed that, among the six crosscutting disciplinary concepts mentioned above, students' reasoning is based on structure-property relationships and benefits-costs-risks. Novice students mostly relied on surface characteristics, familiarity, and their impressions based on real life experiences. On the other hand, advanced students focused on processes, to be more specific, the process of using the fuel. They also focused on the efficiency of the fuel in terms of energy and they considered the impacts on economy and the nature. In terms of structure-property relationships, novice students thought that number of atoms and type of elements composing the fuel determine its properties. Furthermore, novice students thought that shape and size of the molecule and the presence of particular chemical bonds affect the fuel's energy outcome. Advanced students related the properties of the fuel with its submicroscopic characteristics as they were focusing on reaction processes. The authors suggested that in order to help students in applying their knowledge into relevant contexts, teachers should focus on context based learning by creating relevant situations (Banks et al., 2015; Szteinberg et al., 2014).

Chemical mechanism and chemical causality, which are the main foci of this study, refer to how and why chemical reactions happen. Chemical control, on the other hand, is derived from the question "How can chemical processes be controlled?". In order to track students' conceptual progression about chemical mechanism and chemical causality, Yan and Talanquer (2015) conducted a research study targeting undergraduate and graduate chemistry students. Analysis of semistructured interviews with the participants revealed that most of the students tended to think that chemical reactions are initiated by an active agent or an external force. They also thought that chemical reactions are driven by the "needs" of the reactants to become more stable. Results also showed that students mostly lack the dynamic view of chemical reactions. Novice students, for example, explained that chemical reactions occur by simply combination or decomposition of the aggregates without mentioning submicroscopic properties and dynamic processes. However, more advanced students mentioned bond breaking and bond formation processes and some of them mentioned electron transfers and electrostatic interactions among the particles. In another study, undergraduate and graduate students' reasoning while thinking about the reaction process to synthesize a targeted product was investigated (Weinrich and Talanquer, 2015, 2016). Data analysis revealed the conceptual modes that the students held while thinking about the feasibility of chemical reactions to synthesize a targeted product, and these conceptual modes showed various levels of sophistication. Even though explanatory power of the responses improved as students progress through chemistry education, there was not a clear sequence. Similar with the previous research (Yan and Talanquer, 2015), novice students tended to evaluate chemical reactions at macro level by focusing on active reactants, external agents, and physical changes. Even though more advanced students tended to explain chemical processes with submicroscopic and dynamic view, their thoughts about a need for external agents or active compounds still persisted.

Critical analyses of the literature and limited number of empirical studies on students' conceptualization of crosscutting chemistry concepts revealed that students have difficulties in applying chemistry knowledge into relevant contexts due to the traditional instruction lacking interdisciplinary and cross-disciplinary integration of crosscutting concepts in chemistry. Moreover, research on students' conceptual progression about chemical reactions is very limited in terms of sample size and lack of high school students in the sample of empirically driven progressions (Weinrich and Talanquer, 2015, 2016; Yan and Talanquer, 2015). The present study aimed to draw a detailed portrait of reasoning patterns in students' conceptualization of why and how chemical reactions happen for different types of chemical reactions. Different groups of students, namely, high school, undergraduate, and graduate students, participated in this study were selected based on the accumulation of the concepts involving chemical reactions and fundamental concepts that are strongly related with chemical reactions (e.g., chemical bonding, kinetics, chemical equilibrium, and thermodynamics) in the curriculum. Chemical mechanism and chemical causality as two crosscutting disciplinary concepts, play a critical role in chemical thinking and serve as lenses for understanding how students apply and integrate these fundamental concepts into new contexts (i.e., different types of chemical reactions). Findings from the current study may uncover the progression in students' conceptualization of two crosscutting disciplinary concepts which may also affect students' understanding of other chemistry concepts (Weinrich and Talanquer, 2015). Furthermore, mapping students' conceptual progression may uncover how to promote students understanding, develop instructional practices, and make curricular arrangements.

2.4. Students' Understanding of Chemical Reactions

Over several years, students' understanding of chemical reactions and students' alternative conceptions about chemical reactions were investigated by researchers (Barke *et al.*, 2009; Eilks *et al.*, 2007). In this section, research on students' understanding of chemical reactions will be discussed through the lenses of chemical mechanism and chemical causality. Moreover, students' common alternative conceptions about chemical reactions will be summarized.

Various research studies investigated students' understanding of chemical change and how students categorize physical and chemical changes (Ayas and Demirbas, 1997; Calik and Ayas, 2005; Johnson, 2000, 2002; Stavridou and Solomonidou, 1998; Tsaparlis, 2003). Stavridou and Solomonidou (1998) conducted a cross-age (ages 12-18) study with secondary school students to investigate the development of chemical reaction concept across years. Scientific identification of chemical changes increased with the increase of grade levels. Most 14-year-old students focused on macro properties such as gas formation and color changes while identifying chemical reactions. However, some 14-year-old and 16-year-old students distinguished chemical and physical changes focusing on the combination of multiple reactants to form a product. On the other hand, 18-year-olds defined chemical changes in terms of submicroscopic level. They mentioned the changes in the particles of the reactants without relating it to the formation of the product. In the following years, similar studies were conducted with various age groups. For example, in order to investigate how students distinguish chemical and physical changes, Tsaparlis (2003) conducted a research with Grade 10 and first year undergraduate students. It was found that fist year undergraduate students were better at distinguishing chemical and physical changes. However, since students mostly focused on macro properties (e.g., gas formation) they classified evaporation and boiling as chemical change. Another study conducted with Grade 8 students and student teachers revealed that students in both groups relied on observable changes to identify chemical change similar with the previous studies cited above. However, some participants in student teacher group also mentioned that chemical change took place because of bond breaking and bond formations (Calik and Ayas, 2005).

Another body of research investigated how and why chemical processes take place (Ahtee and Varjola, 1998; Ben-Zvi et al., 1987; Boo, 1998; Boo and Watson, 2001; Van Driel et al., 1998). A research study conducted with students from Grade 7, Grade 8, first year senior secondary school, and first year undergraduate levels investigated how students define chemical reactions (Ahtee and Varjola, 1998). Researchers categorized students' responses based on particular criteria. For a response to be acceptable, it should include bond breaking, bond formation, electron transfer in submicroscopic level, and property changes. As grade level progressed, students tended to describe chemical processes in terms of bond breaking and bond formation by mentioning particle interactions in submicroscopic level, contrary to the novice (Grade 7 and Grade 8) students focusing on macroscopic properties while explaining chemical processes. In another study, Boo and Watson (2001) investigated the progression in high school students' understanding of chemical reactions. The authors conducted individual interviews with two groups of students (Grade 12 and Grade 13). Analysis of the interviews revealed a progress in students' understanding of chemical reactions over years. Results showed that students were good at predicting the outcomes of the reactions presented in the interviews. However, students' understanding of reaction energy in terms of supplying or releasing energy and the bond energies was found to be weak. Additionally, students' understanding of reaction process was weak. Their explanations were lacking dynamic view of particle interactions and collisions. Finally, students' explanations regarding driving force of chemical reactions mostly did not include concepts of kinetic and thermodynamic stability. Findings of this research in terms of alternative

conceptions were worth noting. Even though students demonstrated progression in understanding of chemical reactions, various alternative conceptions were held by students from all groups. The most common alternative conception is about the driving force of chemical reactions. Instead of mentioning kinetic and thermodynamic stability, almost all students focused on external agents (e.g., heat, reactive substances, and solvent) as driving force and cause of chemical reactions. Another common alternative conception is that when the ions attract each other, students thought that they form a molecule. Almost half of the students thought that bond breaking is an exothermic process while bond formation is a endothermic process regarding the energy of reactions. Similar number of students held the alternative conception that solvents do not have any role in chemical reactions.

2.5. Summary

This chapter began with explaining constructivist view of learning and conceptual learning in science education. Students come to science classes with preexisting knowledge about the natural phenomena that are to be taught. However, these conceptions may differ from scientifically accepted body of knowledge and therefore may result in building alternative conceptions upon instruction. In order to determine appropriate interventions to promote students' understanding of scientific concepts, researchers have been investigating students' preconceptions and alternative conceptions over several years.

In order to develop research informed curriculum, assessment, and instructional practices it was suggested to investigate students' conceptual progression over several years. Learning progressions, with the same vision, align curriculum, instruction, and assessment practices that revolve around big ideas and crosscutting disciplinary concepts to promote scientific literacy. Similarly, integrating big ideas and crosscutting disciplinary concepts in chemistry education plays a critical role in students' development of chemical thinking. Core ideas related with analysis, synthesis, and transforming matter are seen fundamental for scientific literacy. Based on core practices of chemistry, namely, investigation, design, and evaluation there were six crosscutting disciplinary concepts which were found to be fundamental in chemical thinking. These concepts include chemical identity, structure-property relationships, chemical causality, chemical mechanism, chemical control, and benefits-costs-risks. The main foci of this study were chemical mechanism and chemical causality since there were limited number of empirical studies investigating the progression in students' understanding of these crosscutting disciplinary concepts with limited number of participants.

There were various research studies investigating students' understanding of chemical reactions. Basically, students' identification of chemical change and understanding of chemical processes were investigated by several researchers and it was found that students from multiple age groups tended to identify chemical change based on macroscopic properties, such as gas formation, color change, and explosions. Additionally, some advanced students mentioned the changes of the particle structure in submicroscopic level and mentioned bond breaking and formation processes. While explaining chemical processes, most students had weak understanding of how reactions proceed (e.g., bond breaking, bond formation, and interactions among particles) and energetic factors affecting reactions (e.g., endothermic processes, exothermic processes, kinetic stability, and thermodynamic stability).

Literature survey showed that studies regarding students' understanding of chemical reactions are very limited in terms of sample and in terms of qualitative descriptions of students' reasoning. Mostly, alternative conceptions held by the students were emphasized in the literature. In this respect, this study focused on describing the progression in students' understanding of chemical mechanism and chemical causality in detail and partraying how students apply their knowledge of fundamental chemistry concepts into new contexts (i.e., different types of chemical reactions) through the lenses of chemical mechanism and chemical causality.

3. METHODOLOGY

The main purpose of this study was to map students' conceptual progression of how and why chemical reactions (displacement, decomposition, and combination reactions) happen across different grade levels (Grade 12, Undergraduate 1, Undergraduate 4, and Graduate). In doing so, the study identified the patterns in students' understanding about how and why chemical reactions happen and organized them according to their levels of explanatory power, and consequently explored how students' patterns of understanding about how and why chemical reactions happen change across different grade levels (i.e., different levels of chemistry education). Finally, the study also investigated how students' patterns of understanding change with respect to the type of chemical reaction under analysis. In order to attain these goals, following research questions guided this study:

- (i) How do students' conceptual modes related to chemical mechanism change across different grade levels?
- (ii) How do students' conceptual modes related to chemical causality change across different grade levels?
- (iii) How do students' conceptual modes related to chemical mechanism and chemical causality change with respect to the type of reaction under analysis?

In the following sections, research design, participants and context of the study, instrument and data collection procedures, data analysis, and the strategies adopted to enhance validity and reliability are described in detail, in order to address the research questions.

3.1. Research Design

The research questions mentioned above guided and shaped this research study. Research questions (i) and (ii), required identifying patterns in students' understanding of how and why chemical reactions happen and comparing how these patterns of understanding change across different grade levels (i.e. different levels of chemistry education). In research question (iii), it was aimed to explore how students' understanding about how and why reactions happen depend on the reaction type under analysis. In order to address the research questions, it was required to *explore* and *understand* patterns in students' understanding in a *complete* manner and represent the relationship between them. In other words, to make sense of the meaning that the students derived from the concepts, namely chemical mechanism and chemical causality, a qualitative research approach was adopted (Creswell, 2013).

Among various qualitative approaches, grounded theory was utilized as the research methodology in this study. In grounded theory research, the meaning is derived from the data inductively and substantive theories can be generated (Corbin and Strauss, 2015; Merriam, 2009). In other words, the theory is grounded in the qualitative data (Charmaz, 2006; Merriam, 2009). Grounded theory research is also utilized when there is a need for explaining a process that takes place over a time period. Such processes include education related events and interactions. Grounded theory research requires collecting qualitative data, identifying categories (themes), describing the relationship among these categories, and generating the theory about the process under analysis (Creswell, 2012).

In order to map and track the changes in students' conceptualization of how and why chemical reactions happen across different grade levels, there are two alternative designs, namely, longitudinal and cross-sectional. However, since longitudinal studies depend on collection of data over time, such research study is difficult to conduct due to time restrictions. Alternatively, cross-sectional designs allow researchers to collect data from multiple groups at a single point of time to track a process (Creswell, 2012). Therefore, a cross-sectional design was used in this study, since it allows mapping students' understanding from multiple groups varying in level of chemistry education (Yan and Talanquer, 2015).

3.2. Participants of the Study

Four groups of students participated in this study based on their level of chemistry education (i.e., different grade levels) and milestones in curriculum regarding chemical reactions. These groups included Grade 12 students at high school level, first-year undergraduate students (i.e., freshmen students) majoring in chemistry, fourth-year undergraduate students (i.e., senior students) majoring in chemistry, and graduate students from Master of Science and Doctor of Philosophy programs in chemistry.

A total of 20 participants from high school level (Grade 12) were recruited from four public high schools located in Sariyer and Beşiktaş districts in Istanbul upon presenting permission letter from the directorates of National Education of corresponding districts (see Appendix A). Five students were selected from each high school by their chemistry teachers based on a wide range of achievement in chemistry. Among Grade 12 participants, the gender distribution was almost equal (55% female, 45% male) as it was summarized in Table 3.1. Grade 12 participants were 17-18-year-old college-bound students, intending to study science, engineering, or medicine in the university. During the data collection period, Grade 12 students progressed through chemistry curriculum published in 2013 (MoNE, 2013a). In Grade 9 and Grade 10, the participants involved in Basic Level Chemistry Program, in which students are expected to get familiar with chemistry concepts and symbolic language of chemistry while relating these concepts with everyday life in order to discover the relationship between properties of chemical substances and their functions. Furthermore, they are expected to relate properties of chemical substances and socio-scientific issues (MoNE, 2013a). Then, because Grade 12 participants aimed to pursue career in engineering, medicine, and natural sciences they continued with Advanced Level Chemistry Program in Grade 11 and Grade 12 (MoNE, 2013a). In the Advanced Level Chemistry Program, students get familiar with chemistry concepts, such as structure of atom, laws of thermodynamics, chemical kinetics and chemical equilibrium, and structure-property-usage relationship of chemical substances (MoNE, 2013a). In Grade 9 and 10, the participants had 2 hours of chemistry lessons per week, and in Grade 11 and 12, they studied 4 hours of chemistry per week.

Undergraduate and graduate participants of the study were recruited from the Department of Chemistry in a public research university located in İstanbul. In order to conduct individual interviews with undergraduate and graduate students, a permission letter was obtained from Institutional Review Board for Research with Human Subjects (İNAREK). The permission letter was presented in Appendix A. Undergraduate 1 participant group included 20 students, and the participants were 20 years old on average. This participant group consisted of 17 (85%) female and 3 (15%) male students. During the period of data collection, they were registered in a General Chemistry II course and a corresponding laboratory course, namely Qualitative Analysis. Before these courses, they took General Chemistry I and its corresponding laboratory course, namely Introduction to Practical Chemistry. These courses were required chemistry courses (22 ECTS credits) for Undergraduate 1 chemistry students and they did not take any elective chemistry courses at this stage.

Fourth-year undergraduate students were registered in advanced undergraduate courses such as Physical Chemistry III, Biochemistry, and the related laboratory course at the data collection period. A total of 20 Undergraduate 4 students were participated in this study. Undergraduate 4 group consisted of 15 (%75) female and 5 (%25) male students, and the participants were 25 years old on average. From senior year to this period, Undergraduate 4 students took several required (122 ECTS credits) and elective chemistry courses. The participants took 23 undergraduate chemistry courses on average worth of 119 ECTS credits (on average) during their undergraduate years.

Graduate participants were master and PhD students in chemistry department. Some graduate participants were enrolled in advanced graduate courses in addition to laboratory work, and the others were working toward their theses and dissertations. This participant group included 14 (%82) female and 3 (%18) male graduate students, and they were 29 years old on average. Master students took Advanced Organic Chemistry, Advanced Physical Chemistry, and Graduate Seminar courses in addition to several graduate elective courses. Doctoral students only took a research course as a required course in addition to graduate elective chemistry courses. The participants took 7 graduate chemistry courses on average worth of 47 ECTS credits (on average).

		Gender			
Level of education	Group name	Number of participants	Female	Male	Age
		$n \ (N{=}77)$	f (%)	f (%)	M
Grade 12	G12	20	11 (55)	9(45)	18
Undergraduate 1	UG1	20	17(85)	3(15)	20
Undergraduate 4	UG4	20	15(75)	5(25)	25
Graduate	GR	17	14 (82)	3(18)	29

Table 3.1. Participant demographics.

As it can be seen from the demographic characteristics of the participant groups (see Table 3.1), gender distribution among high school students were almost even. However, the gender distribution of Undergraduate and Graduate groups was female dominant. In order to confirm that this gender distribution reflects the demographic characteristics of the Department of Chemistry, the number of female and male students were obtained and percentage values were computed. Frequencies and percentage values showed that female students outnumber male students in the Department of Chemistry in this particular university. For example, Undergraduate 1 students registered in the Department of Chemistry included 45 female and 23 male, which corresponds to 66% and 34%, respectively. Similarly, 66% of Undergraduate 4 students and 82% of graduate students were female in the Department of Chemistry. When participant demographics and gender distribution in the Department of Chemistry were compared, such participant characteristics in the sample were expected due to the gender distribution in the department that the participants were recruited from. Each participant was identified with a number and in the subsequent chapters, interview excerpts will be labeled with group abbreviation and participant number. For example, seventh participant from Grade 12 is mentioned as G12P7 and 12th participant from Undergraduate 4 group is mentioned as UG4P12.

A total of 77 students, including 20 high school (Grade 12) students, 20 firstyear undergraduate students, 20 fourth-year undergraduate students, and 17 graduate (master/PhD) students volunteered to participate in this study. A total of 20 participants from each group (except the Graduate group) were interviewed until a *saturation* was reached where addition of new data would not change the coding scheme (Charmaz, 2006; Creswell *et al.*, 2007). Students from each group were recruited based on their level of chemistry education and the accumulation of knowledge in chemical reactions throughout the curriculum.

3.3. Context of the Study

In Turkey, there is a centralized core curriculum for high school chemistry course. In 2018, Ministry of National Education published a new chemistry curriculum for high school level (MoNE, 2018). However, Grade 12 students during the data collection period (Spring 2017), progressed through the Turkish chemistry curriculum which was published in 2013 (MoNE, 2013a). Therefore, research context regarding Grade 12 students is represented through the lenses of the chemistry curriculum published in 2013 (MoNE, 2013a). Students are introduced to chemistry as a separate discipline at the first year of secondary education (Grade 9 in high school level) and chemical education continues with Grade 10. Students who aim to pursue career in engineering, medicine, and natural sciences are continued to be taught chemistry in Grade 11 and Grade 12. Chemistry curriculum in the research context includes Basic Level Chemistry Program for Grade 9 and Grade 10 and Advanced Level Chemistry Program for Grade 11 and Grade 12 (MoNE, 2013a). However, both Basic Level Chemistry Program and Advanced Level Chemistry Program mainly focus on developing scientific literacy and science process skills as an outcome of recent curricular reform in Turkey (Erdogan and Koseoglu, 2012). Teaching and learning approaches of the programs include context based chemistry learning in a constructivist learning environment (MoNE, 2013a). However, Demircioglu et al. (2015) stated that even though the chemistry curriculum encourages a constructivist learning environment as a result of curriculum reforms, chemistry teachers avoided reading curriculum and did not change traditional teaching methods in their classrooms. Furthermore, research also showed that teachers did not include classroom activities into their teaching practices, such as laboratory sessions, due to time restrictions (Demir *et al.*, 2017; Demircioglu *et al.*, 2015; Uce and Saricayir, 2013).

In this research context, high school students study chemical reactions from different points of view as they progress through chemistry curriculum. In Grade 9, students are introduced to the concepts of atom, molecule, element, compound, and states of matter. They learn concepts of element and compound as types of chemical substances. Furthermore, they study electrostatic interactions (intra-molecular and intermolecular interactions) and physical and chemical changes on the basis of bond breaking and bond formation. They start to form chemical equations of basic reaction types, namely, combustion, acid-base, and precipitation reactions. In Grade 10. Mixtures unit is dedicated to introduce homogeneous mixtures as solutions and heterogeneous mixtures in detail with an emphasis on the concept of dissolving at the particulate level. Students are also introduced to concepts acid, base, salt, and pH. They discover acid-base reactions as interactions between acids and bases. Furthermore, they learn how acid-base reactions proceed on macro level by focusing on acid-base indicators. In Grade 11, the students are re-introduced to the chemical reactions with a quantitative approach, namely stoichiometry. They are also dealing with the reaction types, namely, combustion, acid-base, precipitation, and redox reactions as well as learning about the basic laws of thermodynamics and spontaneity of chemical reactions. In the *Chemical Kinetics and Equilibrium* unit, Grade 11 students examine chemical reactions in more detail, involving the concepts of molecular collision, activation energy, catalysts, chemical kinetics, reaction mechanisms, chemical equilibrium, acid base definitions, acid-base reactions, and precipitation reactions. In Grade 12, students are introduced to redox reactions and spontaneity of redox reactions in Chemistry and Electricity unit.

In the undergraduate chemistry program, the first-year chemistry students take general chemistry courses (General Chemistry I and General Chemistry II) and the related laboratory courses (Introduction to Practical Chemistry and Qualitative Analysis) separately as required courses. In the second semester general chemistry course, the first-year chemistry students study thermochemistry, thermodynamics, chemical kinetics, chemical equilibrium, acids and bases, solubility, and electrochemistry topics in detail. Both of the general chemistry courses are based on direct instruction and problem solving during lecture hours and problem sessions. Laboratory courses, on the other hand, require students to perform one or more experiments each week and report the results based on a laboratory report template. During the lecture hours of the laboratory courses, students are introduced to the experiments of that week and theoretical knowledge related to the experiments. The participants stated that they do not have discussion sessions about the chemical reactions included in the experiments.

Fourth-year chemistry students take numerous required and elective chemistry courses. In addition to general chemistry courses, fourth-year chemistry students take required courses such as Organic Chemistry I-II-III and related laboratory courses, Inorganic Chemistry with a laboratory course, Physical Chemistry I-II-III with laboratory courses. In addition to the required courses, students take several elective chemistry courses based on their interests. For example, most of the students take more than one undergraduate research courses from several chemistry fields. Among the elective courses that the students take, there are environmental chemistry, textile chemistry, polymer science and technology, and medicinal chemistry. Again, most of the courses they take are based on direct instruction and problem solving.

Master students take Advanced Organic Chemistry, Advanced Physical Chemistry, and Graduate Seminar as required courses. In addition to them, they take six elective graduate chemistry courses based on their research interests and thesis topics. Among these courses, there are Advanced Inorganic Chemistry, Polymer Chemistry, Advanced Computational Chemistry, and special topic courses such as Polymer Composites and Organometallic Chemistry. Doctoral students also take their elective courses from the same pool with the master students. As it can be seen from the courses they take, graduate students start to specialize in chemistry. In addition, they start their laboratory work with their supervisors in addition to the courses until they finish their theses/dissertations.

3.4. Instrument and Data Collection Procedures

Data were collected through semistructured interviews. Interviewing is a procedure in which the participants are asked open ended questions in parallel with the research questions of the study and the answers of the participants are recorded (Creswell, 2012). Since the research questions required participants' in depth explanations, interviews were utilized as the data source. In this study, *individual interviews* (also called *one-on-one interviews*) in which only one participant was interviewed at a single time were adopted (Creswell, 2012). Since targeted information is required from the participants (i.e., chemical mechanism and chemical causality), there were structured questions in the protocol (e.g., How does this reaction start? Why does this reaction happen?). However, the protocol allows probing and elaboration of the ideas for the researcher to explore emerging ideas during the interviews and exact wording was not used in the questions (Merriam, 2009). The interview protocol included four chemical reactions representing various types of chemical reactions, namely double displacement, single displacement, decomposition, and combination. Each of these reactions was chosen by considering their variety in types of chemical bonds, types of physical states, types of substances, and types of driving forces. Furthermore, high school textbooks were scanned and the representative reactions for each type included in this study were selected to ensure their familiarity to the Grade 12 students. The reactions selected for the study were categorized according to the replacement of the particles. Each reaction was presented with their symbolic and particulate representations in the interview protocol. Chemical reactions included in the interview protocol are presented in Table 3.2 and the interview protocol can be seen in Appendix B.

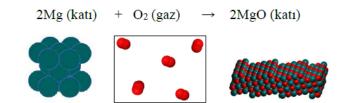
For individual interviews, Grade 12 students were selected by their chemistry teachers based on their achievement in chemistry and their willingness to participate in an interview study at the end of Spring 2017 term. Chemistry teachers were informed about the purposes of the research and the data collection procedures which involves one by one interviews. Since shy and hesitant interviewees cause challenges to the interviewer and they do not express their ideas in detail (Creswell, 2013), the teachers were asked to select students who were willing to share their ideas. Undergraduate and grad-

Type of reaction	Chemical equation
Double displacement	$AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$
Single displacement	$Fe(s) + CuSO_4(aq) \rightarrow FeSO_4(aq) + Cu(s)$
Decomposition	$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$
Combination	$2 Mg(s) + O_2(g) \rightarrow 2 MgO(s)$

Table 3.2. Chemical reactions included in the interview protocol.

uate participants were recruited from the Department of Chemistry in a public research university located in İstanbul. The first-year undergraduate students were recruited through an announcement during a general chemistry laboratory course hour at the end of Spring 2017 and Spring 2018 semesters. The fourth-year undergraduate participants were invited during an undergraduate seminar course and an undergraduate physical chemistry course (Physical Chemistry III) in Fall 2017 semester. Furthermore, an invitation e-mail was sent to all senior chemistry students by their academic advisor. The graduate students were recruited via e-mail invitations and through announcements in chemistry laboratories in Fall 2017 and Spring 2018 semesters.

Before the individual interviews, the participants were informed about the purpose of the research and they were informed that their responses would be used only for research purposes. The researcher stated that their participation in this study would not affect their grades and that they can withdraw from the study anytime without penalty. In addition, they were informed that right or wrong answers were not interested by the researchers. Rather, the participants were encouraged to express their thinking during interview tasks in detail. Then, they were asked to fill out the demographic information forms, which are different for high school and undergraduate/graduate students (see Appendix C and Appendix D).



d. Aşağıda gördüğünüz kimyasal reaksiyonda magnezyum katısı oksijen gazı ile tepkimeye girerek magnezyum oksit oluşturmaktadır.

- Görmüş olduğunuz tepkime sizce nasıl başlamıştır?
- Tepkimeye giren maddeleri düşündüğünüzde, tepkimeyi başlatan bir madde olduğunu düşünüyor musunuz? Neden?
- Tepkime sürecini/mekanizmayı çizebilir misiniz? Çizdiğiniz mekanizmayı açıklayınız.
- Görmüş olduğunuz tepkime sizce neden gerçekleşmiştir?
- Görmüş olduğunuz tepkime sizce ne zaman sona ermektedir?

Figure 3.1. An example representation used in the interview protocol

Because the interview protocol included colored representations, each reaction was shown on a computer screen one by one. The participants were shown particulate and symbolic representations of each chemical reaction. First, each participant classified the reaction under analysis. Then the participants were asked to explain how the reaction under analysis starts and proceeds. Then, they were asked to explain why the reaction under analysis happens. They were also asked to support their explanations with drawings, if possible. Thus, they were provided with pencil, paper, and periodic table. Participants' drawings and interview transcripts were merged later for a better understanding of their responses. Finally, the participants were asked when the reaction would stop. An example of the representations given in the interview protocol can be seen in Figure 3.1. The participants were encouraged to think aloud while answering the questions. The participants were asked probing questions in order to explore their thinking about chemical reactions under analysis in detail. Probing questions, which are subquestions under each of the interview questions, allow the interviewee to express his/her ideas in detail in order to obtain *clarity* and *elaborate* his/her ideas (Creswell, 2012). The participants' responses to the main interview questions shape the probing questions during the interviews (Merriam, 2009). The following interview excerpt demonstrates how the reactions (e.g., $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$) were introduced to the participants:

Researcher: "[...] This is the third reaction. Here [in the visual] we see calcium carbonate. Calcium carbonate reacts to produce calcium oxide and carbon dioxide gas. Let's start with the type of this reaction." UG1P8: "[...] Decomposition reaction... Carbon dioxide leaves the medium in a gas form while calcium oxide remains as a solid." Researcher: "[...] Okay, how do you think this reaction starts and proceeds?"

Interviews were conducted in a proper place in participants' schools (e.g., libraries, laboratories, offices, meeting rooms, and classrooms). The individual interviews took between 30 and 60 minutes, and they were audio-recorded and transcribed verbatim for analysis. In order to understand the participants' explanations better, their drawings were scanned and integrated with the corresponding transcription parts.

3.5. Data Analysis

The major data source of this research study was the transcripts of individual interviews. In order to address the research questions, individual interviews were transcribed verbatim. Then, qualitative analyses were performed. In this section, data analysis procedures will be explained in detail.

In order to analyze the data, interview transcripts were read, reread, and coded initially. Coding of the transcripts allowed the researcher to understand the data deeply (Charmaz, 2006). For coding process, NVivo qualitative data analysis software, version 11 was used. Charmaz (2006) defined coding as categorizing pieces of the data and naming them with labels that summarize these pieces. In coding process, naming pieces of the data (initial coding) was followed by a more focused coding phase in which the data were organized, synthesized, and integrated (Charmaz, 2006). During the coding process, *constant comparative method* was utilized. In constant comparative method, pieces of data were coded, and new codes emerged or the data fit into an existing code. During the coding process, each piece of data that was coded was compared with the other data coded under the same category (Glaser and Strauss, 1967). In this research context, this process was applied within the same transcript (the responses of the same participant) and among all of the transcripts (the responses of all participants). As the properties of the codes emerged, some codes were integrated and some of them were eliminated (Glaser and Strauss, 1967). In other words, coding process was shaped by the addition of the new codes, as the data analysis progressed. Constant comparative method of analysis proceeded iteratively with simultaneous data collection and analysis. Data collection and analysis processes continued until a *saturation* was reached where new addition of data would not change the coding scheme (Charmaz, 2006; Creswell *et al.*, 2007).

In the current context, students' conceptual progressions were investigated under two concepts, namely chemical mechanism and chemical causality. For each concept, the following dimensions emerged:

- (i) Concept: Chemical mechanism (How do chemical reactions happen?)
 - Dimension: How chemical reactions start
 - Dimension: How chemical reactions proceed
 - Dimension: When chemical reactions stop
- (ii) Concept: Chemical causality (Why do chemical reactions happen?)
 - Dimension: Why chemical reactions happen
 - Dimension: What causes chemical reactions
 - Dimension: What drives chemical reactions

These dimensions and categories emerged for each dimension were named by utilizing the scheme developed in the previous studies (Weinrich and Talanquer, 2015; Yan and Talanquer, 2015). However, as it was mentioned in the previous paragraphs, coding scheme was modified by addition, elimination, and integration of the codes as the data collection and data analysis progressed. In this study, each code (category) emerged under these dimensions are named *conceptual mode* as suggested by the previous studies (Weinrich and Talanquer, 2015; Yan and Talanquer, 2015). For example, for the dimension "when chemical reactions stop", some participants assumed that chemical reactions would stop when all reactants were consumed. Such way of conceptualization was categorized under "when reactants are gone" conceptual mode. On the other hand, some participants assumed that chemical reactions would not stop. Instead, competing processes would keep going as a dynamic equilibrium. Such conceptualization of the participants was categorized under "dynamic equilibrium" conceptual mode. Conceptual modes under each dimension were arranged according to the sophistication and explanatory power. For each reaction, frequency and percentage of participants holding such conceptual modes were calculated and represented as visual models (see Chapter 4). In addition, dimensions and conceptual modes under analysis were depicted visually in the following chapter (see Chapter 4).

The rest of this section was dedicated to explain concepts of chemical causality and chemical mechanism. Additionally, related dimensions and conceptual modes were defined and described with corresponding coding keys in detail in Sections 3.5.1 and 3.5.2.

3.5.1. Chemical Mechanism: How do Chemical Reactions Happen?

Sevian and Talanquer (2014) suggested investigating the progression in students' conceptions of *cross-cutting disciplinary concepts* considered as fundamental in chemistry understanding and practice. These concepts involve chemical identity, structure–property relationships, chemical causality, chemical mechanism, chemical control, and benefits–costs–risks. This study focused on two of these concepts, namely, chemical mechanism and chemical causality. The question "How do chemical reactions happen?" targets the concept of chemical mechanism. In the context of this study, this concept consists of three dimensions, namely, how chemical reactions start, how chemical reactions proceed, and when chemical reactions stop.

The first dimension *how chemical reactions start* focuses on the participants' conceptions of how different types (i.e., double displacement, single displacement, decomposition, and combination) of chemical reactions start. Participants' responses under this dimension were categorized into five conceptual modes as shown in the Table 3.3.

Table 3.3. Coding key for the conceptual modes regarding "how chemical reactions

at art"	
start	٠

Conceptual modes	Description
Just happens	Chemical reactions happen spontaneously or when the reac-
	tants are mixed
Active agent	The reactant with more reactivity, mobility or electronegativ-
	ity starts the reaction
External forces	External forces (e.g., heat, light) starts the reaction
Mutual attraction	Chemical reactions start by the electrostatic attraction be-
	tween particles of the reactants
Random collisions	Chemical reactions start when the particles of the reactants
	collide with each other

Table 3.4. Coding key for the conceptual modes regarding "how chemical reactions proceed"

Conceptual modes	Description
Combination of aggregates	Reactions are combination of the particles of the
	reactants
Displacement of aggregates	Reactions are displacement of particles of the re-
	actants
Decomposition of aggregates	Reactions are decomposition of a reactant
Bonds broken and reformed	Chemical bonds are broken and reformed to pro-
	duce the product
Changes through interactions	As chemical bonds are broken and reformed, elec-
	tron transfer and/or electrostatic interactions take $% f(x)=f(x)$
	place

Table 3.5. Coding key for the conceptual modes regarding "when chemical reactions stop".

Conceptual modes	Description
When reactants are gone	Chemical reactions stop when the reactants are
	consumed
When external force is removed	Chemical reactions stop when the external force is
	removed
Stops at equilibrium	Chemical reactions stop at equilibrium
Dynamic equilibrium	The reaction never stops, dynamic equilibrium
	continues

The dimension of *how chemical reactions proceed* classifies participants' conceptual modes according to their responses about how the particles of reactants of different types of chemical reactions interact to form the targeted products. Five conceptual modes emerged from participants' responses regarding this dimension. Explanations of the conceptual modes were summarized in Table 3.4.

When chemical reactions stop dimension classifies participants' conceptual modes according to their responses about when no more chemical changes are observed. Participants' conceptual modes regarding this dimension were summarized in Table 3.5.

3.5.2. Chemical Causality: Why do Chemical Reactions Happen?

The question "Why do chemical reactions happen?" targets the concept of chemical causality. In this research context, this concept is classified into three dimensions, namely, why chemical reactions happen, what causes chemical reactions, and what drives chemical reactions. The dimension of *why chemical reactions happen* is categorized into six conceptual modes based on participants' responses regarding the reasons and necessary conditions behind chemical changes. The conceptual modes emerged under this dimension were described in Table 3.6.

The dimension of *what causes chemical reactions* categorizes participants' responses about how properties and interactions of the particles involved in chemical changes affect these processes. Furthermore, this dimension involves external agents (e.g., heat, electricity, catalysts) that influence chemical reactions.

Table 3.6. Coding key for the conceptual modes regarding "why chemical reactions happen".

Conceptual modes	Description
Active agent	Reactions happen due to the reactant with more reac-
	tivity or electronegativity
External forces	Reactions happen due to the external forces (heat, light)
Attractive forces	Reactions happen due to the strong electrostatic attrac-
	tions between the particles of reactants
Teleological explanations	Reactions happen due to the needs or wants of the par-
	ticles of the reactants
Causal explanations	Reactions happen due to the reactants' features which
	affect their interactions
Probability	Reactions happen due to the random interactions of par-
	ticles of the reactants

Table 3.7. Coding key for the conceptual modes regarding "what causes chemical reactions".

Conceptual modes	Description
Central agent	Reactions are driven or caused by one central agent
	(e.g., heat or a reactive substance)
Multiple agents in sequence	Reactions are driven or caused by two or more reac-
	tant or agents acting sequentially
Multiple interacting agents	Reactions are driven or caused by multiple interacting
	agents (concomitant mutual interactions)

The last dimension regarding chemical causality is *what drives chemical reactions*. This dimension categorizes participants' responses regarding whether chemical processes are driven by energetic or entropic factors based on the changes in Gibbs energy (Muller, 1994). Three conceptual modes emerged under this dimension were described in Table 3.8.

Table 3.8. Coding key for the conceptual modes regarding "what drives chemical reactions".

Conceptual modes	Description
Energy driving	Reactions are driven by only energetic factors
Energy-entropy merged	Reactions are driven by both energetic and entropic
	factors, but some alternative conceptions included
	in the explanations regarding distinguishing between
	energy and entropy concepts
Energy and entropy driving	Reactions are driven by both energetic and entropic
	factors

3.5.3. Interpreting the Data

Findings from this study are presented in Chapter 4. Conceptual modes emerged for chemical mechanism and chemical causality are described qualitatively along with representative interview excerpts given in the separate tables dedicated to each dimension. Then, frequency and percentages calculated for the expressions of the conceptual modes are presented in tables for all educational levels.

In order to address the research questions (i) and (ii), the conceptual modes expressed for a particular dimension for all reaction were added and divided by the total conceptual modes expressed for the dimension under analysis (see Section 4.1). Then, the ratios were transformed into percentages. Table 3.9 represents the distribution of the conceptual modes for a particular dimension. In order to provide a clear expression and to prevent any confusion with the hypothetical data and the actual conceptual modes, the hypothetical dimension given in Table 3.9 is called "dimension 1" and the hypothetical conceptual modes given in the table are named "Conceptual mode 1", "Conceptual mode 2", and "Conceptual mode 3". The data represented in Table 3.9 are hypothetical as well. Hypothetical conceptual modes and the data are given to provide a clear understanding of how frequencies and percentages of the expressed conceptual modes were calculated.

Table 3.9. Hypothetical representation of the conceptual modes regarding "dimension1" across different grade levels.

Conceptual modes	G12 (n=20)	UG1 $(n=20)$	UG4 $(n=20)$	GR $(n=17)$
	f~(%)	f~(%)	f~(%)	f (%)
Conceptual mode 1	12 (60)	6(33)	14(47)	3(15)
Conceptual mode 2	6(30)	5(28)	10(33)	7(35)
Conceptual mode 3	2(10)	7(39)	6 (20)	10 (50)
Total	20 (100)	18 (100)	30 (100)	20 (100)

As it can be seen from Table 3.9, UG1 column shows that 6 of 20 students in the group expressed "Conceptual mode 1", 5 of 20 students expressed "Conceptual mode 2", and 7 of 20 students expressed "Conceptual mode 3". Out of 20 students of UG1 group, 18 conceptual modes are expressed in total for "dimension 1". This indicates that there are some students that do not have any response regarding "dimension 1". On the other hand, UG4 column shows that, 14 of 20 students expressed "Conceptual mode 1", 10 out of 20 students expressed "Conceptual mode 2", 6 out of 20 students expressed "Conceptual mode 3". This distribution shows that some students expressed more than one conceptual mode for "dimension 1". GR column also shows that there are students expressed more than one conceptual mode for "dimension 1". Percentage values are calculated for a particular student group by computing total frequencies of the conceptual modes for "dimension 1".

In order to address the research question (iii), the percentages of the conceptual modes for each educational level for a single reaction type were calculated (see 4.2). Therefore, total frequencies of the conceptual modes for each group are calculated for the reaction under analysis. Since the reactions were investigated one by one, for some conceptual modes, there existed only one or two explanations. In order to obtain a meaningful description of the distributions of the conceptual modes, total frequencies of the conceptual modes were divided by the number of participants. Then, the ratios were transformed into percentages. In order to enhance clarity, frequencies of students providing no response were represented in the corresponding tables. Because the percentages were calculated by using the number of participants, total percentages exceeded 100% if some students expressed more than one conceptual modes for some dimensions.

3.6. Validity and Reliability in Qualitative Research

Regarding the validity and reliability of qualitative research, various terminologies, definitions, and validation procedures were proposed by several authors (Creswell, 2013; Merriam, 2009). It should be noted that underlying philosophical assumptions of qualitative research designs differ from quantitative approaches. Therefore, definitions of validity and reliability should be in alignment with such philosophical assumptions, which have different views on reality (Merriam, 2009).

Several authors use the term *validity* for trustworthiness and credibility of qualitative research designs and consider validity as a goal which depends on the purposes of the research study and the research questions (Creswell, 2013; Creswell and Miller, 2000; Merriam, 2009). It can be defined as how accurately participants' reality about the phenomena under analysis is represented (Creswell and Miller, 2000). On the other hand, *reliability* of qualitative research designs is referred as the stability of the data to various coders. In the following paragraphs, the procedures used in order to enhance validity and reliability of this research study were discussed.

3.6.1. Validation Strategies Utilized in the Study

In this research study, terminologies and validation procedures were adopted from various authors (Creswell, 2013; Creswell and Miller, 2000; Merriam, 2009). Validation is defined as the procedures used by the researchers in order to enhance the credibility of the research study (Creswell and Miller, 2000).

<u>3.6.1.1. Triangulation.</u> In this validation strategy, various sources of data, multiple researchers, or theories can be used to generate categories and codes (Creswell, 2013; Creswell and Miller, 2000; Merriam, 2009). In this study, the only data source was the interview transcripts. In constant comparative analysis of the data, participant responses corresponding each of the categories (conceptual modes) were compared for the whole sample. Furthermore, within the transcript of a single participant, the responses were compared for each category, for each reaction under analysis. This comparison allowed the researcher to synthesize, eliminate, or separate the codes. In addition, the coding process for the whole sample was performed with another researcher (thesis supervisor) and the codes and the instances were compared to ensure that the same meaning for each code was driven by the researchers.

<u>3.6.1.2.</u> Adequate Engagement in Data Collection. This validation strategy requires spending adequate time with data collection until saturation is reached (Merriam, 2009). In this study, data collection and data analysis procedures applied simultaneously in order to reach various categories and the cases that invalidate the categories until a saturation is established. Such cases were reported in detail in Chapter 4.

<u>3.6.1.3.</u> Clarifying Researcher Bias. This validation strategy is also called *researcher* reflexivity (Creswell and Miller, 2000). This strategy requires the researcher to establish and describe her assumptions, biases, and position that may shape the research process (Creswell, 2013; Creswell and Miller, 2000; Merriam, 2009). In this study, researcher's perspectives and theoretical orientation that shaped her interpretation were discussed in chapters dedicated to the theoretical framework of the study, literature review, research context, and discussion related to this study (see Chapters 1, 2, 3, and 5).

<u>3.6.1.4. Thick, Rich Descriptions.</u> This validation strategy requires the researcher to describe the characteristics of the research context, characteristics of the participants, and codes in detail (Creswell, 2013; Creswell and Miller, 2000; Merriam, 2009). Such detailed descriptions help the readers feel that they are familiar with the research context, the participants, and the participants' experiences about the phenomenon under investigation. Moreover, thick and rich descriptions allow the readers to decide whether the characteristics described in the research are similar to their situations. This helps the readers to decide whether they can transfer the findings described in the research study to their situation or to similar contexts. In order to enhance validity from this perspective, context of the research, the curriculum and the learning environment that the participants are involved, data collection procedures and environment, and the participant characteristics were described in detail in Chapter 3.

<u>3.6.1.5. Maximum Variation.</u> Finally, variation and diversity in sample characteristics were recommended by Merriam (2009). This helps the readers to transfer the findings to the various situations and contexts, a purpose which is similar to the *thick, rich descriptions* strategy. In order to enhance validity with this strategy, participants were

tried to be selected from various educational backgrounds (for Grade 12 participants, various high schools) and a range of academic achievement (see Sections 3.2 and 3.3).

Creswell (2013) recommends using at least two validation strategies for a qualitative research study. For this research, triangulation, adequate engagement in data collection, clarifying researcher bias, maximum variation, and thick, rich descriptions were used, since these strategies were suitable for the research design and data collection procedures which involves individual interviews with a high number of participants.

3.6.2. Enhancing Reliability in the Study

As it was mentioned before, reliability in qualitative research designs refers to the stability of the data to the various coders (Creswell, 2013). Therefore, in order to enhance reliability, inter-coder agreement was adopted in this study. Inter-coder agreement requires multiple coders to analyze the data.

In the current research, the data source was individual interview transcripts. Inter-coder agreement was determined in terms of percent agreement as suggested by Miles and Huberman (1994). First, 15% of the total transcripts were randomly selected. There were 77 transcripts in total, so 12 transcripts were recoded by the researcher and another researcher (thesis supervisor) separately. First, total codes in agreement were counted. In order to determine the codes in agreement, code names and the passages that were coded were compared. Then, total number of codes were counted (i.e., total number of agreements + disagreements) as given in Equation 3.1. Total codes in agreement were divided by the total number of codes.

$$reliability = \frac{number \ of \ agreements}{total \ number \ of \ agreements + \ disagreements}$$
(3.1)

Finally, the ratio was transformed into the percentage value. As a result, 95% agreement was obtained in the current study. Miles and Huberman (1994) suggested that inter-coder agreement should reach 90%. Therefore, inter-coder agreement obtained in the current study can be considered as satisfactory.

4. FINDINGS

Constant comparative analysis of the data revealed the dimensions and conceptual modes regarding the concepts of *chemical mechanism* and *chemical causality*. The following dimensions emerged for each concept:

(i) Chemical mechanism: How do chemical reactions happen?

- Dimension: How chemical reactions start
- Dimension: How chemical reactions proceed
- Dimension: When chemical reactions stop
- (ii) Chemical causality: Why do chemical reactions happen?
 - Dimension: Why chemical reactions happen
 - Dimension: What causes chemical reactions
 - Dimension: What drives chemical reactions

Figure 4.1 represents the conceptual modes regarding each dimension which are ordered in increasing level of sophistication. Conceptual modes that are judged to be equal in terms of sophistication are given in the same box. Even though this map demonstrates the conceptual modes expressed by the participants of this study in an increasing manner from left to right, it does not indicate a linear increase in sophistication of the conceptual modes.

Data analysis showed that expression of the conceptual modes by the participants depended both on the level of chemistry education and the type of reaction under consideration. Students' expressions of the conceptual modes depended on the grade level for all reaction types, when the reactions were examined one by one. Descriptions of reaction process regarding *chemical mechanism* and all dimensions of *chemical causality* depended on the level of chemistry education for all reaction types. These dimensions are given as following:

- How chemical reactions proceed
- Why chemical reactions happen
- What causes chemical reactions
- What drives chemical reactions

Progression in students' understanding of chemical reactions will be explained in detail in Section 4.1. Description of how students' expression of the conceptual modes depended on the type of reaction under consideration will be presented in Section 4.2.

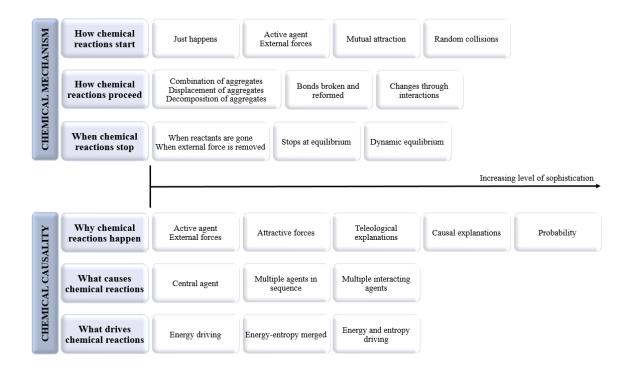


Figure 4.1. Dimensions and conceptual modes regarding chemical mechanism and chemical causality

4.1. Students' Conceptual Progression of Chemical Reactions

In order to address research questions (i) and (ii), this section firstly described conceptual modes identified for all grade levels in detail. Secondly, conceptual progression and patterns in students' understanding of how and why chemical reactions happen across different levels of chemistry education were described in detail with frequencies and percentage values in corresponding tables. The research questions addressed in this section are:

- Research Question (i): How do students' conceptual modes related to chemical mechanism change across different grade levels?
- Research Question (ii): How do students' conceptual modes related to chemical causality change across different grade levels?

4.1.1. Chemical Mechanism

Chemical mechanism, as a crosscutting disciplinary concept, connected to the question "How do chemical reactions happen?". Regarding this concept, three dimensions emerged, namely, how chemical reactions start, how chemical reactions proceed, and when chemical reactions stop. Subsequent paragraphs describe students' conceptual modes and conceptual progressions regarding chemical mechanism in detail.

<u>4.1.1.1. How Chemical Reactions Start.</u> The dimension how chemical reactions start focuses on the participants' conceptions of how different types of chemical reactions (i.e., double displacement, single displacement, decomposition, and combination) start. Analysis of students' explanations revealed five types of conceptual modes, namely, *just happens, active agent, external forces, mutual attraction, and random collisions.* These conceptual modes are shown in Table 4.1 with illustrative excerpts from the individual interviews in increasing levels of sophistication.

Table 4.2 demonstrates the frequencies and percentage values of the conceptual modes expressed by the different groups of students for all reaction types. The most expressed conceptual modes regarding *how chemical reactions start* for all groups was *active agent* and *external forces*. The conceptual mode *active agent* based on students' explanations including chemical reactions start by an active agent which has more activity, more mobility (e.g., atoms of a gas), or electronegativity (e.g., chloride ions). This conceptual mode was expressed mostly by Grade 12 (28.9%), Undergraduate 4 (29.6%), and Graduate students (31.8%), and it was less frequently observed among

UG1 students (20.3%). Moreover, student responses coded as *external forces* included expressions such as chemical reactions are started by external forces such as heat and electricity. This conceptual mode was expressed frequently by students from all groups, but it was more frequent among Grade 12 (44.7%) and Undergraduate 1 (49.4%) students, and it was less frequent among Undergraduate 4 (37.0%) and Graduate (39.4%) students.

reactions start [*] .			
Conceptual modes	Interview excerpts		
Just happens	G12P1: "A precipitation reaction occurs here. Silver and		
	chloride combined and precipitated. Then, this structure is		
	formed [] sodium and nitrate."		
Active agent	GR1P3: "We need to consider the activity of metals [] iron		
	has higher activity than copper. Therefore, iron displaced copper."		
External forces	UG1P13: "In order to break apart the molecule, in order to		
	break the bonds, there is a need for energy. In order to give		
	energy we supply heat."		
	UG1P6: "[] in order to break apart magnesium, we need		
	something like a catalyst, we need heat."		
Mutual attraction	UG4P19: "When we mix the solutions, silver and chloride		
	ions combine due to ionic attraction between them. Because		
	of the strong attraction between them, water can not separate		
	them."		
Random collisions	GRP5: "Free ions are moving in the water constantly $[\ldots]$ In		
	the water, there are collisions and movements of the molecules		
	towards each other $[\ldots]$ As a result of the constant movement		
	of the particles, silver and chloride combine and start to form		
	a precipitate. When we stir the solution, the precipitate would		
	form faster because of the increase in collision rate."		

Table 4.1. Interview excerpts for the conceptual modes regarding "how chemical reactions start".

Conceptual modes	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
Just happens	4(5.3)	0 (0.0)	0 (0.0)	0 (0.0)
Active agent	22 (28.9)	16(20.3)	24 (29.6)	21 (31.8)
External forces	34(44.7)	39(49.4)	30 (37.0)	26 (39.4)
Mutual attraction	15(19.7)	22 (27.8)	21 (25.9)	15(22.7)
Random collisions	1(1.3)	2(2.5)	6 (7.4)	4(6.1)

 Table 4.2. Frequencies of conceptual modes regarding "how chemical reactions start"

 across different grade levels.

Some students in the sample demonstrated superficial understanding regarding how chemical reactions started. These students stated that chemical reactions *just happen* when reactants are mixed or when reactants are present in the same medium. Most of these students focused on the macro properties of the substances while explaining the initiation of the chemical reactions. For example, they stated that precipitation formation is observed when the reactants are mixed or a slow oxidation process (rusting) may occur when magnesium is left in an open container. This conceptual mode was expressed only by a limited number of Grade 12 students (f=4, 5.3%) when thinking about double displacement and combination reactions.

The most frequent conceptual modes regarding how chemical reactions start expressed by the students were active agent and external forces. The participants who expressed the conceptual mode of active agent stated that a chemical that acts as an active agent (e.g., particles with more electronegativity and particles with more mobility) starts chemical reactions. The majority of participants expressed this conceptual mode when thinking about single displacement reaction, which included electron transfer process as well. Regarding the single displacement reaction, the participants focused on the activity of the metals as it can be seen from the Table 4.1. Participants also expressed this conceptual mode when thinking about the double displacement reaction and combination reaction as well. Considering the double displacement reaction, the participants focused on the agent which had high electronegativity (e.g., chloride ion). While considering the combination reaction, participants focused on the particle which had higher mobility (e.g., oxygen gas). This conceptual mode was expressed mostly by Graduate (31.8%) and Undergraduate 4 (29.6%) students. It was expressed less frequently by Undergraduate 1 (20.3%) and Grade 12 (28.9%) participants. Conceptual mode of *external forces* was the most frequently expressed conceptual mode among all grade levels (for *how chemical reactions start* dimension). This conceptual mode indicated that chemical reactions started when an external agent was introduced to the reaction medium. These external agents can be heat, flame, or electricity. While considering the decomposition reaction, the participants expressed only the conceptual mode of *external forces* when thinking about the starting process. In addition, the majority of the participants expressed this conceptual mode while thinking about the combination reaction. This conceptual mode was expressed mostly by undergraduate 1 (49.4%) and Grade 12 (44.7%) students. It was expressed less frequently by Undergraduate 4 (37.0%) and Graduate (39.4%) participants.

Conceptual mode of *mutual attraction* indicated that chemical reactions start when the particles of reactants attract each other through electrostatic interactions to form the targeted products. Data analysis showed that this conceptual mode was expressed mostly when thinking about the double displacement reaction. It was also expressed when students were explaining the single displacement reaction. When compared with *active agent* and *external forces*, it was less frequently expressed and it was mostly expressed by Undergraduate and Graduate students. Among students at university level, Undergraduate 1 (27.8%) and Undergraduate 4 (25.9%) students expressed the conceptual of *mutual attraction* mode more than the Graduate students (22.7%).

Finally, few number of participants expressed the conceptual mode of *random* collisions while thinking about how chemical reactions start. This conceptual mode indicated that particles of the reactants are in a constant motion and collide each other with various energies and orientations. When these collisions occur with enough kinetic energy and with proper orientations, chemical reactions start. Similar to the

other conceptual modes, expression of this conceptual mode depended on the chemical reaction under analysis. Participants expressed this conceptual mode only when thinking about the double displacement reaction taking place in an aqueous medium and the combination reaction involving a solid metal and a gas. It was expressed mostly by Undergraduate 4 students (7.4%) followed by Graduate (6.1%) students. While only one out of 20 Grade 12 students and two of 20 Undergraduate 1 students expressed this conceptual mode when thinking about the double displacement reaction. Students' expressions of the conceptual modes for each type of reaction were described in detail in Section 4.2.

<u>4.1.1.2. How Chemical Reactions Proceed.</u> The dimension how chemical reactions proceed focuses on the participants' conceptions of how the particles of reactants of different types of chemical reactions (i.e., double displacement, single displacement, decomposition, and combination) interact to form the targeted products. Analysis of students' explanations revealed five types of conceptual modes, namely, combination of aggregates, displacement of aggregates, decomposition of aggregates, bonds broken and reformed, and changes through interactions. These conceptual modes are shown in Table 4.3 with illustrative excerpts from the individual interviews in an increasing level of sophistication.

Data analysis showed that students' explanations of the conceptual modes regarding how chemical reactions proceed depended on the type of reaction under analysis and the level of chemistry education. Frequencies and percentages of the conceptual modes expressed for this dimension are presented in Table 4.4. It appeared that the participants with higher level of chemistry education (e.g., Undergraduate 4 and Graduate participants) tended to express conceptual modes with higher explanatory power (e.g., bonds broken and reformed and changes through interactions) when thinking about the chemical processes. Grade 12 and Undergraduate 1 students, on the other hand, tended to describe chemical processes in terms of *combination/displacement/decomposition of aggregates* by stating that chemical reactions proceed as the particles of reactants combine, replace each other, or break apart to produce the targeted products.

Table 4.3. Interview excerpts for the conceptual modes regarding "how chemical reactions proceed"

Conceptual modes	Interview excerpts
Combination of ag-	UG4P17: "When we mix silver nitrate and sodium chloride so-
gregates	lutions, we will see a white precipitate in a crystal form at the
	bottom [] We know that silver nitrate and sodium chloride
	are soluble. When silver and chloride attract each other as plus
	and minus ions, they will form a precipitate because they are
	insoluble."
Displacement of ag-	UG1P6: "Iron displaces copper while donating its electrons be-
gregates	cause it is more active than copper [] Copper will precipitate
	in an elemental form. Iron two plus will form $FeSO_4$ compound,
	and the color of a solution will change."
Decomposition of ag-	G12P17: "Heat helps the decomposition of them $[CaCO_3]$
gregates	molecules]. It breaks apart the bonds between the molecules."
Bonds broken and	GRP7: "Carbonate is a covalently bonded ion which has an ionic
reformed	interaction with calcium ion. When we heat it it decomposes
	into carbon dioxide and O^{-2} . Then, Ca^{+2} and O^{-2} attract each
	other."
	$C_{2}^{(2)} = $
Changes through in-	GRP7: "Silver and chloride ions are freely moving in the so-
teractions	lution. Due to the electrostatic attraction between them, they
	move towards each other and water molecules can not separate $\$
	them $[\ldots]$ At the same time, water-nitrate and water-sodium in-
	teractions will remain. Therefore, sodium and nitrate ions will
	remain in the solution."

Conceptual modes	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
Combination of aggregates	27 (35.5)	29(36.7)	25(32.1)	13(18.8)
Displacement of aggregates	22 (28.9)	18(22.8)	13(16.7)	11(15.9)
Decomposition of aggregates	17(22.4)	8 (10.1)	9(11.5)	3(4.3)
Bonds broken and reformed	3(3.9)	17(21.5)	12(15.4)	21(30.4)
Changes through interactions	7(9.2)	7(8.9)	19(24.4)	21 (30.4)

Table 4.4. Frequencies of conceptual modes regarding "how chemical reactions proceed" across different grade levels.

More than half of the conceptual modes expressed by Grade 12, Undergraduate 1, and Undergraduate 4 participants accumulated on *combination of aggregates, displacement of aggregates*, and *decomposition of aggregates*. These conceptual modes were judged to have similar explanatory power since they are all similar in terms of expressing the particles of reactants as aggregates combining, replacing, or breaking apart depending on the reaction type. In other words, the difference showed itself based on the nature of chemical reaction under consideration. For example, conceptual mode of *displacement of aggregates* was expressed only when students were thinking about the decomposition reaction. Participants who expressed this conceptual mode stated that the reaction proceeded as the particles of reactant break apart into simpler molecules. On the other hand, conceptual mode of *combination of aggregates* was expressed when thinking about the double displacement reaction which involved a precipitation process and the combination reaction. Finally, conceptual mode of *displacement of aggregates* was expressed when thinking about the double and single displacement reactions.

Conceptual mode of *bonds broken and reformed* indicated that chemical reactions proceed as the chemical bonds of the reactants break apart and new chemical bonds are formed while producing the products. Participants usually considered chemical processes several sequential events while expressing this conceptual mode. For example, the participants sequenced the events in a reaction as following: heating bond breaking - bond formation - product formation. This conceptual mode expressed mostly when thinking about the decomposition and combination reactions. Only one of 17 Graduate students expressed this conceptual mode when describing the single displacement reaction. As it can be seen from the Table 4.4, this conceptual mode was mostly expressed by Undergraduate and Graduate students. Among the university level students, this conceptual mode was mostly expressed by the Graduate students (30.4%). The Graduate students were followed by 21.5% of Undergraduate 1 and 15.4% of Undergraduate 4 students who expressed *bonds broken and reformed* while describing the chemical processes. Expression of the conceptual mode increased with increasing level of chemistry education. Even though there seemed to be decrease in Undergraduate 4 group, it can be seen that their responses were accumulated in *changes through interactions* in among the conceptual modes with higher explanatory power.

Some participants, especially the ones in high grade levels, described chemical reactions in terms of the properties of the particles affecting the reaction process and interactions of the particles. Such explanations of the reaction processes were coded as *changes through interactions*. As it can be seen in Table 4.4, expression of this conceptual mode increased as students progressed through chemistry education. Expression of this conceptual mode was almost equal between Grade 12 (9.2%) and Undergraduate 1 (8.9%) students. A dramatic increase was observed in the expression of this particular conceptual mode, such as Undergraduate 4 (24.4%) and Graduate (30.4%). This conceptual mode was expressed when students think about double displacement, single displacement, and combination reactions.

<u>4.1.1.3.</u> When Chemical Reactions Stop. The dimension when chemical reactions stop focuses on the participants' conceptions of when different types of chemical reactions (i.e., double displacement, single displacement, decomposition, and combination) would stop. Analysis of students' explanations revealed four types of conceptual modes, namely, when reactants are gone, when external force is removed, stops at equilibrium, and dynamic equilibrium. These conceptual modes are shown in Table 4.5 with illustrative excerpts from the individual interviews in increasing levels of sophistication.

Data analysis showed that expressions of the conceptual modes by the students based on the level of chemistry education and the reaction type under analysis. Table 4.6 demonstrates the frequencies and percentage values of the conceptual modes expressed by the students for all reaction types. Majority of the explanations regarding when chemical reactions stop accumulated on the conceptual modes when reactants are gone and when external force is removed.

	reactions stop".
Conceptual modes	Interview excerpts
When reactants are gone	G12P5: "This reaction stops when oxygen or magnesium
	is consumed. If they are given equally, the reaction stops
	when both of them are consumed."
	UG4P13: "The reaction stops when carbon dioxide for-
	mation is completed."
When external force is	UG1P8: "When we stop heating, the reaction would
removed	stop, because we need energy to break the bonds."
	GRP1: "Because this reaction is not spontaneous, it
	would stop when we stop giving energy."
Stops at equilibrium	UG4P9: "The reaction stops when it reaches chemical
	equilibrium. When ion concentrations reach equilibrium
	constant, it stops."
Dynamic equilibrium	G12P4: "This reaction doesn't stop. Precipitation and
	dissolving processes keep going on."
	GRP9: "I think this reaction wouldn't stop [] electron
	transfer would keep going on between iron and copper
	[] for example, iron ions and copper ions would be
	present in the solution."

Table 4.5. Interview excerpts for the conceptual modes regarding "when chemical

Conceptual modes	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
When reactants are gone	70 (76.1)	75(78.9)	63 (75.9)	62(72.9)
When external force is removed	14(15.2)	16(16.8)	10(12.0)	18 (21.2)
Stops at equilibrium	2(2.2)	3(3.2)	9(10.8)	1(1.2)
Dynamic equilibrium	6(6.5)	1(1.1)	1(1.2)	4(4.7)

Table 4.6. Frequencies of conceptual modes regarding "when chemical reactions stop" across different grade levels.

Conceptual modes of when reactants are gone and when external force is removed were judged to be having the similar complexity in terms of explanatory power. Conceptual mode of when reactants are gone refers to the explanations stating that chemical reactions stop when all reactants or limiting agent are consumed. In addition, it refers to the statements expressing that the reactions stop when all products are formed. While mentioning the formation of the products, the participants focused on the macroscopic evidences, such as "when the gas formation stops" or "when the precipitate formation stops". For the reactions including heating (e.g., decomposition and combination reactions) the participants also expressed the conceptual mode of when external force is removed by stating that the reactions would stop if the external force (e.g., heat) is withdrawn from the reaction medium. These conceptual modes were expressed by the majority of the participants from all educational levels. Percentages and frequencies of the expressions of these conceptual modes can be seen in Table 4.6.

Conceptual mode of *stops at equilibrium* referred to explanations stating that chemical reactions stop when a certain equilibrium constant is reached or when the substances reached certain concentrations (e.g., molarities). This conceptual mode was expressed when thinking about double displacement, single displacement, and decomposition reactions. It was expressed mostly by Undergraduate 4 students (10.8%). What made this conceptual mode different from *dynamic equilibrium* was that conceptual mode of *stops at equilibrium* does not include the particulate level explanations, indicating that backward and forward reactions occur simultaneously. Here, it was stated that the reactions would stop even though an equilibrium state was mentioned. On the other hand, conceptual mode of *dynamic equilibrium* indicated that chemical reactions would not stop and considered dynamic process of backward and forward reactions. *Dynamic equilibrium* was mostly expressed when thinking about double displacement reactions. Some participants expressed this conceptual mode when they think about single displacement and decomposition reactions as well. It was expressed mostly by Grade 12 (6.5%) and Graduate (4.7%) students. When compared with *when reactants are gone* and *when external force is removed*, expression of these conceptual modes were quite rare for all educational levels.

4.1.2. Chemical Causality

Chemical causality, as a crosscutting disciplinary concept, connected to the question "Why do chemical reactions happen?". Regarding this concept, three dimensions emerged, namely, why chemical reactions happen, what causes chemical reactions, and what drives chemical reactions. Subsequent paragraphs describe students' conceptual modes and conceptual progressions regarding chemical causality in detail.

<u>4.1.2.1.</u> Why Chemical Reactions Happen. The dimension why chemical reactions happen focuses on the participants' conceptions regarding the reasons and necessary conditions behind different types of chemical reactions (e.g., double displacement, single displacement, decomposition, and combination). Analysis of students' explanations revealed six types of conceptual modes, namely, active agent, external forces, attractive forces, teleological explanations, causal explanations, and probability. These conceptual modes are shown in Table 4.7 with illustrative excerpts from the individual interviews in increasing levels of sophistication.

Table 4.7. Interview excerpts for the conceptual modes regarding "why chemical

reactions ha	appen".
--------------	---------

Conceptual modes	Interview excerpts
Active agent	G12P8: "This reaction happens due to the activity of the
	metals. Activity of iron leads to electron transfer."
External forces	UG1P16: "This reaction occurs because we are giving
	energy to the system."
Attractive forces	G12P9: "Usually ions form ion-dipole interactions with
	water and they dissolve [] Water molecules surround
	plus and minus ions. However, when silver and chloride
	interact with each other, water molecules are not strong
	enough to separate and dissolve them."
Teleological explanations	UG1P11: "Why this reaction happens Because
	When we give energy to the system, they [magnesium
	and oxygen] prefer forming bonds with each other to be-
	come more stable."
Causal explanations	UG4P9: "Both of them [iron and copper] have empty d
	orbitals. This allows electron transfer between them. As
	a result of the electron transfer, they form more stable
	products."
Probability	GRP5: "Free ions are moving in the water constantly
	[] In the water, there are collisions and movements
	of the molecules towards each other. For example, even
	though silver nitrate dissolve in water, they have mo-
	mentary interactions. We can see them interacting in a
	t moment. As a result of the constant movement of the
	particles, silver and chloride combine and start to form
	a precipitate. When we stir the solution, the precipitate
	would form faster because of the increase in collision
	rate."

Data analysis revealed that participants' expressions regarding *why chemical reactions happen* accumulated on the conceptual modes of *active agent*, *external forces*, and *attractive forces*. Explanation of the conceptual modes with more explanatory power depended on educational level. Frequencies and percentage values of the conceptual modes regarding *why chemical reactions happen* can be seen in Table 4.8.

Conceptual modes	G12	UG1	UG4	GR
	f(%)	f (%)	f (%)	f (%)
Active agent	20 (30.3)	23 (31.5)	25(32.5)	24(37.5)
External forces	16(24.2)	28 (38.4)	17(22.1)	13(20.3)
Attractive forces	22 (33.3)	18 (24.7)	20 (26.0)	12 (18.8)
Teleological explanations	4 (6.1)	2(2.7)	9 (11.7)	2(3.1)
Causal explanations	4(6.1)	2(2.7)	5(6.5)	12 (18.8)
Probability	0 (0.0)	0 (0.0)	1(1.3)	1(1.6)

Table 4.8. Frequencies of conceptual modes regarding "why chemical reactions happen" across different grade levels.

Conceptual modes of *active agent* and *external forces* were considered having similar explanatory power. Conceptual mode of *active agent* emerged for double displacement reaction, single displacement reaction, and combination reaction. In the double displacement reaction, this conceptual mode refers that chemical reactions happen because of presence of an active agent which has more electronegativity (e.g., chloride ion). On the single displacement reaction, it refers that the reactions happen due to the presence of an active agent which has more activity (i.e., activity of metals). On the combination reaction it refers to the presence of an agent which has more mobility (e.g., oxygen gas). Conceptual mode of *external forces* was expressed when explaining the reasons behind the decomposition and combination reactions. While expressing this conceptual mode, the participants stated that the reaction happened due to introducing heat or another type of energy source to the reaction medium. In other words, the participants stated that the reaction happened because it was forced to happen by the external agents. More than half of the participants from all groups expressed these two conceptual modes when explaining *why chemical reactions happen*.

Conceptual mode of *attractive forces* was among the most expressed conceptual modes by the participants. It was mentioned mostly when explaining the double displacement reaction. It was also expressed while describing the reasons behind the other three types of chemical reactions (i.e., single displacement, decomposition, and combination) even though the frequencies were relatively low (see Tables 4.16, 4.18, and 4.20). Conceptual mode of *attractive forces* refers that the reactions happen due to the electrostatic interactions between particles of the reactants as seen in Table 4.7. This conceptual mode was expressed mostly by Grade 12 students (33.3%), and it was less frequent among the Graduate students (18.8%).

Conceptual modes of *teleological explanations* and *causal explanations* were mostly expressed by the students with higher educational level (e.g., Undergraduate 4 and Graduate). Students who utilized *teleological explanations* stated that the reactions happen due to the wants, urges, or needs of the substances. In other words, students attributed human characteristics (e.g., to want and to need) to the chemical substances. When the reaction types were examined one by one, it was found that conceptual mode of *teleological explanations* was expressed for all reaction types. The students who stated *teleological explanations* focused on substances' needs for being thermodynamically and/or kinetically stable or their need for being in a lower energy state. Such explanations were observed mostly among the Undergraduate 4 students (11.7%). It was less frequent among Undergraduate 1 (2.7%) and Graduate (3.1%)students. Conceptual mode of *causal explanations*, on the other hand, focuses on the features of the reactants as reasons behind chemical reactions. Even though it was mostly expressed when explaining the decomposition reaction, it was mentioned for all reaction types. While expressing this conceptual mode, the participants refer to the energetic and/or kinetic stability of the substances mostly by referring to their properties instead of their wants and needs. This conceptual mode was frequently expressed by the Graduate students (18.8%).

Finally, conceptual mode of *probability* indicates that chemical reactions happen due to the random collisions and interactions of the particles. A total of two students, one from Undergraduate 4 group and one from Graduate group, expressed this conceptual mode when explaining double displacement and combination reactions, respectively (see Tables 4.14 and 4.20).

<u>4.1.2.2. What Causes Chemical Reactions.</u> The dimension what causes chemical reactions focuses on how properties and interactions of the particles involved in different types pf reactions affect these chemical processes. Furthermore, this dimension involves external agents (e.g., heat, electricity, catalysts) that influencing chemical reactions. Analysis of students' explanations revealed three types of conceptual modes, namely, *central agent, multiple agents in sequence, and multiple interacting agents.* These conceptual modes are shown in Table 4.9 with illustrative excerpts from the individual interviews in increasing levels of sophistication. Frequencies and percentages regarding the conceptual modes are given in Table 4.10.

Data analysis showed that more than half of the Grade 12 (64.3%) and Undergraduate 1 (81.3%) students thought that a *central agent* affects chemical processes and makes them keep going. This central agent could be an external agent such as heat, or particles of the reactants. Type of the central agent that the participants were referring to depended on the reaction type. For example, for the decomposition reaction of CaCO₃, some participants expressed that heat makes the reaction keep going. They stated that the reaction would not continue if one stopped heating the reaction medium. For the displacement reaction of Fe and CuSO₄, the participants expressed that iron, as an active metal, makes the reaction keep going. Expression of this conceptual mode was less frequent among the Undergraduate 4 (40.8%) and Graduate students (46.7%).

Table 4.9. Interview excerpts for the conceptual modes regarding "what causes

	chemical reactions".
Conceptual modes	Interview excerpts
Central agent	G12P20: "At the beginning, these atoms are bonded to-
	gether. In order to make carbon dioxide leave the reac-
	tion medium in a gas form, these bonds need to break
	apart. There is a need for energy to break the bonds []
	and energy is needed to make this reaction keep going.
	We supply energy to this reaction by heating."
Multiple agents in se-	GRP16: "Because magnesium is a metal, it is able to
quence	donate its free electrons when we give energy. When it
	donates its electrons to oxygen, the bonds between oxy-
	gen atoms will be broken and magnesium oxide will be
	formed. Similarly, second oxygen atom will do the same
	with another magnesium atom. At the end, two magne-
	sium oxide molecules will be formed."
Multiple interacting	GRP3: "When we mix two solutions [silver nitrate and
agents	sodium chloride solutions], silver and chloride attract
	each other because of the strong interactions between
	them. Water molecules don't have enough attractive
	forces to separate these ions. Interactions between water
	molecules and silver ions and interactions between wa-
	ter and chloride ions are weaker than the interactions
	between silver and chloride ions. Therefore, when silver
	and chloride ions attract each other, they don't separate
	and therefore, form a precipitate. Even though sodium
	and nitrate ions attract each other, the interaction be-
	tween these ions is weaker than the interaction between
	the water molecules and these ions [sodium and nitrate
	ions]. Therefore, water molecules can separate them and
	they remain in the solution."

When thinking about the factors affecting the chemical processes, some participants expressed that *multiple agents in sequence* make the reactions keep going. While expressing this conceptual mode, participants put multiple events in a sequence in the reaction process as it can be seen in the example given in Table 4.9. This conceptual mode was expressed mostly by Undergraduate 4 (22.4%) and Graduate (33.3%) participants when thinking about decomposition, and combination reactions. Furthermore, some participants expressed this conceptual mode when thinking about the single displacement reaction.

Conceptual mode of *multiple interacting agents* includes students' explanations claiming that the reactions are affected and driven by multiple agents (i.e., particles) interacting to form the targeted products. During their explanations, students explicitly mentioned the dynamic nature of the reaction media and expressed how properties of the particles affected the reaction process as they are in constant interaction (see Table 4.9). This conceptual mode was expressed mostly by the Undergraduate 4 students (36.7%) followed by the Graduate students (20.0%) while analyzing the double displacement reaction. Some students also mentioned this conceptual mode while explaining single displacement and combination reactions as well.

Conceptual modes	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
Central agent	18(64.3)	26 (81.3)	20 (40.8)	28 (46.7)
Multiple agents in sequence	6(21.4)	2(6.3)	11(22.4)	20 (33.3)
Multiple interacting agents	4(14.3)	4(12.5)	18(36.7)	12 (20.0)

Table 4.10. Frequencies of conceptual modes regarding "what causes chemical reactions" across different grade levels.

<u>4.1.2.3. What Drives Chemical Reactions.</u> The dimension what drives chemical reactions focuses on participants' responses regarding energetic and entropic drivers of different types of chemical reactions (i.e., double displacement, single displacement, decomposition, and combination). Analysis of students' explanations revealed three types of conceptual modes, namely, *energy driving*, *energy-entropy merged*, and *energy and entropy driving*. These conceptual modes are shown in Table 4.11 with illustrative excerpts from the individual interviews in increasing levels of sophistication.

Data analysis showed that explanations of the conceptual modes regarding *what drives chemical reactions* depended on the level of chemistry education. Furthermore, it is important to note that only one of 20 Grade 12 students provided explanations regarding this dimension. Frequencies and percentages of the conceptual modes can be seen in Table 4.12.

Half of the Undergraduate 1 students, 38.5% of Undergraduate 4 students, and 39.1% of Graduate students expressed the conceptual mode of *energy driving* regarding energetic and entropic drivers of chemical reaction. This conceptual mode was expressed for all reaction types, but mostly for combination reaction and decomposition reactions. Participants who expressed this conceptual mode focused on kinetic and/or thermodynamic stability of the particles as well as reactions' status in terms of being endothermic or exothermic.

Conceptual mode of *energy-entropy merged* was the least expressed conceptual mode among the three (i.e., energy driving, energy-entropy merged, and energy and entropy driving). It was expressed mostly by Undergraduate 4 students (23.1%) among the Undergraduate and Graduate participants. Almost equal number of students expressed this conceptual mode among Undergraduate 1 (16.7%) and Graduate (17.4%) participants. When thinking about energetic and entropic drivers of chemical reactions, the participants who expressed this conceptual mode had alternative conceptions regarding energy and entropy terms or they used these terms interchangeably as it can be seen from the example in Table 4.11. In the example given in Table 4.11 an Undergraduate 4 participant stated that:

UG4P15: "When silver and chloride ions collide and precipitate, they form a more stable product. They form a solid [...] Entropy is decreasing here, so this reaction is favorable." - (Energy-entropy merged)

In the representative interview excerpt given above, the participant expressed that the reaction was favorable, because there was a decrease in entropy. However, before this explanation, he stated that the precipitate was a more stable product. One can interpret that this participant used entropy and energy terms interchangeably or had an alternative conception regarding the relationship between spontaneity of the reactions and entropy changes.

 Table 4.11. Representative interview excerpts for the conceptual modes regarding

 "what drives chemical reactions".

	what drives chemical reactions.
Conceptual modes	Interview excerpts
Energy driving	GRP12: "In order to form calcium oxide and carbon
	dioxide we need to give energy to the system. After we
	give energy to the system, the energy of the products
	is higher than the energy of the reactants. Because we
	supplied heat"
Energy-entropy	UG4P15: "When silver and chloride ions collide and
merged	precipitate, they form a more stable product. They form
	a solid $[\ldots]$ Entropy is decreasing here, so this reaction
	is favorable."
Energy and entropy	GRP7: "Because of the gas formation, entropy of the
driving	reaction increases which is a favorable process. On the
	other hand, there is a bond formation and bond break-
	ing. A pi bond is formed and a sigma bond is broken.
	Because sigma bond is stronger, we need to give energy
	to the system, which is an unfavorable process. Since
	ΔG is affected by ΔH minus $T\Delta S$, these two processes
	are competing."

Finally, some students considered both energetic and entropic factors as drivers of the chemical reactions by expressing the conceptual mode of *energy and entropy driving.* This conceptual mode was mostly expressed by the Graduate students (43.5%) and frequently by Undergraduate 4 participants (38.5%). This conceptual mode was expressed for all reaction types, but it was most frequently expressed for the decomposition reaction. Participants who expressed this conceptual mode focused on both energetic and entropic factors by considering Gibbs free energy and its equation ($\Delta G = \Delta H - T\Delta S$) as it can be seen from the interview excerpt of GRP7 given in Table 4.11. This conceptual mode was expressed for all reaction types as well, but it was mostly expressed for the decomposition reaction.

 Table 4.12. Frequencies of conceptual modes regarding "what drives chemical reactions" across different grade levels.

Conceptual modes	G12	UG1	UG4	GR
	f (%)	f(%)	f(%)	f(%)
Energy driving	0 (0.0)	9 (50.0)	5(38.5)	9 (39.1)
Energy-entropy merged	0 (0.0)	3(16.7)	3(23.1)	4 (17.4)
Energy and entropy driving	1(5.0)	6(33.3)	5(38.5)	10(43.5)

4.2. Students' Conceptual Progression of Chemical Reactions Based on the Type of Reaction Under Analysis

In order to address the research question (iii), students' expressions regarding chemical mechanism and chemical causality were presented based on the reaction types under analysis. The research question addressed in this section is: "How do students' conceptual modes related to chemical mechanism and chemical causality change with respect to the type of reaction under analysis?" Data analysis revealed that students' conceptual modes for chemical mechanism and chemical causality differed with respect to the reaction types and the level of chemistry education. In order to demonstrate the common patterns in students' explanations, the classification categories were first represented in tables for each reaction type. Then, conceptual modes emerged for each type of reaction were represented in the corresponding tables.

4.2.1. Double Displacement Reaction

As a representative of double displacement reactions, the participants were given the reaction between silver nitrate (AgNO₃) and sodium chloride (NaCl). In this reaction, the ions constantly move and collide with water molecules and with each other resulting in the displacement of the ions to produce NaNO₃ and AgCl. When, for example, Na⁺ and NO₃⁻ collide, their interactions with the water molecules overcome their interactions with each other. Therefore, they remain in the solution. However, when Ag⁺ and Cl⁻ ions collide with proper orientation and energy, interactions of the ions overcome their interactions with water molecules. As a result, they form a strong electrostatic attraction resulting in separation from the solution as a solid aggregate. The formation of this precipitate as an ionic lattice is an exothermic process, in which products have lower energy than the reactants. There is a decrease in the entropy of the system since ions move away from solution to the lattice. Therefore, it can be concluded that this reaction is energetically driven.

Frequencies and percentages of classification categories in participants' expressions were given in Table 4.13. Analysis of participants' classifications revealed that most of the Grade 12 and more than half of the Undergraduate students tended to classify this reaction as a precipitation reaction. Frequency of *precipitation* category decreased dramatically in the expressions of Graduate participants. More than half of the Graduate participants classified this reaction as a displacement reaction while 18% of the Graduate participants expressed that this was a precipitation reaction. The frequency of expressing *displacement* category seemed to increase as the participants progress through chemistry education. As the grade level increased, the participants' focus shifted from the surface features to the particle arrangements; for example, 40% of Undergraduate 4 and 71% of Graduate participants seemed to focus on the arrangement of the particles while classifying this reaction.

Classification categories	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
Displacement	0 (0)	2(10)	6(30)	10(59)
Precipitation	14(70)	11 (55)	11 (55)	3(18)
Displacement and precipitation	2 (10)	7(35)	2(10)	2(12)
Other	4 (20)	0 (0)	1(5)	2(12)
Total	20 (100)	20 (100)	20 (100)	17(100)

 Table 4.13. Frequencies of classification categories regarding double displacement

 reaction across different grade levels.

Data analysis showed that the dimensions how chemical reactions start, how chemical reactions proceed, why chemical reactions happen, what causes chemical reactions, and what drives chemical reactions seemed to depend on the level of chemistry education for double displacement reaction. Conceptual modes emerged for double displacement reaction were given in Table 4.14.

The participants' expressions regarding how chemical reactions start for the double displacement reaction seemed to change with respect to the level of chemistry education. Only a limited number of Grade 12 students (f=3, 15%) expressed conceptual mode of *just happens*, specifying that this reaction started when the reactants were in the same medium. The most expressed conceptual mode among all participants was *mutual attraction*, indicating that this reaction started with the mutual interactions of the ions. Following interview excerpts demonstrate the conceptual modes having less explanatory power:

G12P17: "Here, silver chloride precipitates. The other [NaNO₃] still dissolves. It starts with displacement of the ions. It is their own property." - (Just happens) G12P12: "For example, in periodic table, when we get closer to fluorine, reactivity

increases. For metals, reactivity increases as we move from top to the bottom. Maybe these two [Ag and Cl ions] are so reactive that they can combine and form a precipitate." - (Active agent)

The conceptual mode of *mutual attraction* emerged mostly from the responses of Undergraduate 4 (75%), Graduate (70%) and Undergraduate 1 (70%) students. On the other hand, expressing the conceptual mode of random collisions increased with respect to the level of chemistry education. The participants who expressed this conceptual mode focused on the constant, random motion of the ions in the solution and their constant electrostatic interactions. The conceptual mode *active agent* which had less explanatory power than *mutual attraction* and *random collisions* was expressed mostly by Grade 12 students. The distribution of the conceptual modes among the grade levels showed that all Graduate participants expressed the conceptual modes with higher explanatory power (i.e., mutual attraction and random collisions). The Undergraduate 1 (80%) and Undergraduate 4 (90%) participants mostly expressed the conceptual modes with higher explanatory power as well, but it seemed that some participants in both groups expressed that the presence of an active agent (e.g., particle with higher electronegativity) started this reaction. The Grade 12 students, on the other hand, mostly focused on the presence of an active agent (25%) in the reaction medium as a starter and mutual electrostatic interactions among the ions (55%). Following examples illustrate the expressions of conceptual modes having more explanatory power:

UG4P7: "I can say that strong attraction between silver and chloride starts this reaction [...] Plus and minus charges stick together [..] and they create strong intermolecular forces." - (Mutual attraction) GRP8: "The particles keep colliding. When they keep interacting and as silver and chloride keeps colliding, they attract each other." - (Random collisions)

The participants' expressions regarding how chemical reactions proceed for the double displacement reaction mostly included *combination of aggregates* for all levels of chemistry education. The conceptual modes regarding *how chemical reactions proceed* demonstrated similar characteristics among Grade 12 and Undergrad 1 students (see Table 4.14). They mostly thought that double displacement reaction proceeded as the particles of the reactants combined to form a precipitate. Additionally, some Grade 12

students (f=3, 15%) stated that particles of the reactants replace each other to form the products. Even though conceptual mode of *combination of aggregates* was dominant among Undergraduate 4 and Graduate participants, some participants' expressions shifted to a more dynamic view indicating that chemical reactions proceed by the dynamic interactions of the ions and water molecules in the reaction medium. In other words, conceptual mode of *changes through interactions* seemed to be expressed mostly among Undergraduate 4 (35%) and Graduate (29%) students. The following interview excerpts demonstrated the increase in sophistication of the conceptual modes regarding the reaction mechanism:

UG1P9: "[...] When we add silver nitrate solution into sodium chloride solution, silver and chloride will attract each other due to their plus and minus charges. When we mix the solutions, they combine and precipitate. This does not take place between sodium and nitrate ions because they will not precipitate." - (Combination of aggregates)

G12P15: "Silver and sodium will displace and silver chloride will be formed." - (Displacement of aggregates)

GRP7: "Silver and chloride ions are freely moving in the solution. Due to the electrostatic attraction between them, they move towards each other and water molecules can not separate them [...] At the same time, water-nitrate and water-sodium interactions will remain. Therefore, sodium and nitrate ions will remain in the solution." - (Changes through interactions)

While thinking about when double displacement reaction stops, the majority of all groups expressed that this reaction stops when the reactants are consumed or when the formation of precipitation stops. Following excerpt illustrates the conceptual mode of *when reactants are gone*:

UG1P10: "The reaction stops when the reactants are consumed. Or.. When the limiting reactant is consumed. It depends on the amount of the reactants." -(When reactants are gone)

While 20% of Undergraduate 4 students thought that the reaction stops at equilibrium (e.g., when a certain equilibrium constant is reached), 20% of Grade 12 (f=4) and 18% of Graduate (f=3) students expressed a process of dynamic equilibrium in which the precipitation formation and ionization occurred simultaneously. The following examples show the conceptual modes of stops at equilibrium and dynamic equilibrium:

UG4P17: "Reactions continue until concentrations of silver and chloride decreases to a certain degree. I think the reaction does not finish, I can not collect all reactants as silver chloride. The probability of interactions [of silver and chloride ions] will decrease as the concentrations decrease." - (Stops at equilibrium) GRP6: "Since there is an equilibrium state here, silver chloride will keep dissolving and precipitating." - (Dynamic equilibrium)

The participants' explanations regarding why double displacement reaction happened seemed to focus on the conceptual mode of *attractive forces* for all levels of chemistry education. Their explanations revealed that double displacement reaction occurred due to the attractive forces among the ions. Following example shows the most expressed conceptual mode, namely *attractive forces*:

G12P1: "There is a strong ionic bond [between silver and chloride]. Therefore, they [water molecules] can not separate the ions. Other ions [sodium and nitrate] remain in the water and they can not form ionic bonds." - (Attractive forces)

However, some participants' explanations seemed to have more explanatory power, stating that double displacement reaction happened due to the chemical properties of the particles which affected their interactions. Such explanations (*i.e., causal explanations*) were found in the responses of Undergraduate 4 and Graduate students. The explanations concerning the conceptual mode of *causal explanations* were low (f=2, 10%) among Undergraduate 4 students. When students progressed to Graduate level, their expressions of these conceptual modes increased slightly. Expressing the conceptual mode of *causal explanations* increased to 18% in Graduate (f=3) group. Furthermore, only one student from Graduate group explained that double displacement reaction took place due to the random interaction of the particles. Following example illustrate the conceptual mode of *causal explanations*:

GRP4: "Silver chloride is more stable than silver nitrate. Because they are all ions, they are in the solution. However, silver chloride and sodium nitrate are more stable than the reactants [...] By using the term stable, I mean that they have lower energy." - (Causal explanations)

reaction across different grade levels.					
Conceptual modes	G12	UG1	UG4	GR	
	f (%)	f (%)	f (%)	f (%)	
How chemical reactions start					
Just happens	3(15)	0 (0)	0 (0)	0 (0)	
Active agent	5(25)	3(15)	4(20)	0 (0)	
Mutual attraction	11 (55)	14(70)	15(75)	12 (70)	
Random collisions	1 (5)	2(10)	3(15)	4 (24)	
No response	0 (0)	1(5)	0 (0)	1(6)	
How chemical reactions proceed					
Combination of aggregates	14 (70)	18 (90)	12(60)	10 (59)	
Displacement of aggregates	3(15)	0 (0)	1 (5)	2 (12)	
Changes through interactions	2(10)	2(10)	7(35)	5(29)	
No response	1(5)	0 (0)	0 (0)	0 (0)	
When chemical reactions stop					
When reactants are gone	15 (75)	18 (90)	16 (80)	14 (82)	
Stops at equilibrium	1 (5)	1(5)	4(20)	0 (0)	
Dynamic equilibrium	4(20)	1(5)	0 (0)	3 (18)	
No response	0 (0)	0 (0)	0 (0)	0 (0)	
Why chemical reactions happen					
Active agent	2(10)	1(5)	2(10)	1(6)	
Attractive forces	17 (85)	16(80)	17 (85)	11 (64)	
Teleological explanations	1 (5)	0 (0)	2(10)	0 (0)	
Causal explanations	0 (0)	0 (0)	2(10)	3 (18)	
Probability	0 (0)	0 (0)	0 (0)	1(6)	
No response	0 (0)	3(15)	0 (0)	1(6)	
What causes chemical reactions					
Central agent	0 (0)	5(25)	2(10)	3 (18)	
Multiple interacting agents	4(20)	4(20)	$13 \ (65)$	9(53)	
No response	16(80)	11 (55)	5(25)	5 (29)	
What drives chemical reactions					
Energy driving	0 (0)	1(5)	1 (5)	1(6)	
Energy-entropy merged	0 (0)	1 (5)	1(5)	0 (0)	
Energy and entropy driving	0 (0)	3(15)	0 (0)	2 (12)	
No response	20 (100)	15(75)	18 (90)	14 (82)	

Table 4.14. Frequencies of conceptual modes regarding the double displacement reaction across different grade levels

While thinking about the properties and interactions of the particles affecting the double displacement reaction, the participants mostly focused on *multiple interacting agents*. This conceptual mode was expressed mostly among Grade 12, Undergraduate 4, and Graduate students. However, only four of 20 Grade 12 students provided an explanation regarding this dimension, and all of them expressed the conceptual mode of *multiple interacting agents*. Other than Grade 12 students, Undergraduate 4 and Graduate students thought that the double displacement reaction was affected by the mutual interactions among the particles (e.g., ions and water molecules). Among these two groups, the percentage of expressing this conceptual mode was higher in Undergraduate 4 group (65%). The 25% of Undergraduate 1 students thought that the double displacement reaction was an ion with higher electronegativity. The number of conceptual modes expressed by Undergraduate 1 students was low when compared with Undergraduate 4 and Graduate participants. Explanations of the conceptual modes can be seen in the following examples:

UG4P20: "Chlorine has high electronegativity. Therefore, it attracts silver strongly [...] There are no other particles with high electronegativity to separate silver from chlorine. For example, nitrate can not separate silver because chlorine has high electronegativity." - (Central agent)

UG4P3: "Ions need to move and collide. They have vibration and translation energies. Therefore, they can form chemical bonds. To form chemical bonds, they need to collide with proper orientation, geometry, and active regions and reach activation energy." - (Multiple interacting agents)

For the double displacement reaction, expression of conceptual modes regarding the driving forces of the reaction was quite low for all grade levels. As a matter of fact, only Undergraduate and Graduate participants provided explanations regarding energetic and entropic drivers of the double displacement reaction. While three of 20 Undergraduate 1 (15%) and two of 17 Graduate (12%) participants were expressing that the double displacement reaction was driven by both energetic and entropic factors, the Undergraduate 4 participants focused on only energetic factors (f=1, 5%) or used energy and entropy terms interchangeably (f=1, 5%). Students' explanations can be seen in the following interview excerpts: UG1P7: "This reaction is spontaneous because the products have less energy." - (Energy driving)

UG4P15: "The products will be more stable... There is a solid formation. Therefore, entropy is decreasing. It is favorable due to the decrease in entropy." - (Energyentropy merged)

UG1P19: "Due to precipitation formation, disorder decreases. Therefore, entropy decreases as well [...] This is an exothermic reaction and delta G is smaller than zero. It is negative... As a result, the reaction is favorable." - (Energy and entropy driving)

4.2.2. Single Displacement Reaction

As a representative of single displacement reactions, the participants were given the reaction between iron (Fe) and a copper sulphate solution (CuSO₄). In this reaction, iron displaces copper. During this process, electron transfer takes place between iron atoms and copper ions. Therefore, this reaction can be classified as a redox reaction as well. Constant movement of the ions in the solution and vibrations of iron lead to random collisions of the particles. When they collide in proper orientation and energy to overcome the activation barrier, electron transfer takes place between Fe atoms and Cu²⁺ ions. This electron transfer leads to formation of Fe²⁺(aq) ions and Cu (s) metal. As the solid copper forming, Fe²⁺ and SO₄²⁻ ions remain in the solution, because the electrostatic interactions between the ions are weaker than their interactions with water molecules. This reaction is an exothermic process in which energy is released from the system to the surroundings.

Frequencies and percentages of classification categories in participants' expressions were given in Table 4.15. Analysis of participants' classifications revealed that half of the Grade 12 participants classified this reaction as a *redox* reaction. Only a small number of Grade 12 participants expressed that this was a *displacement* reaction (10%) and both displacement and redox reaction (15%). The majority of Undergraduate 1 students (65%) classified as both *displacement and redox* reaction. For Undergraduate 4 and Graduate participants, there was not a dominant classification category. Data analysis showed that while Grade 12 participants focused on *redox* when classifying this reaction, Undergraduate participants focused on both *displacement and redox*. Graduate participants, on the other hand, were almost evenly distributed among displacement, redox, and displacement and redox categories.

Data analysis showed that the dimensions of how chemical reactions proceed, when chemical reactions stop, why chemical reactions happen, what causes chemical reactions, and what drives chemical reactions seemed to depend on the level of chemistry education for the single displacement reaction. Conceptual modes emerged for the single displacement reaction were given in Table 4.16.

Table 4.15. Frequencies of classification categories regarding single displacement reaction across different grade levels

Classification categories	G12	UG1	UG4	GR
	f (%)	f (%)	f~(%)	f (%)
Displacement	2(10)	3(15)	5(25)	5(29)
Redox	10 (50)	3(15)	7(35)	6 (35)
Displacement and redox	3(15)	13 (65)	7(35)	4 (24)
Other	5(25)	1(5)	1(5)	2(12)
Total	20 (100)	20 (100)	20 (100)	17 (100)

When thinking about the single displacement reaction, most of the participants stated that the reactant with more activity (e.g., iron) or the reactant with the tendency to receive electrons (e.g., copper) started this reaction. These explanations were coded as *active agent* meaning that the more active agent started the chemical reaction. The majority of the participants (65%, 80%, 70%, and 59% of G12, UG1, UG4, and GR groups, respectively) classified this chemical process as a redox reaction. Therefore, they considered the initiation of electron transfer process while thinking about a redox reaction. Following excerpt shows the expression of conceptual mode, called *active agent*.

GRP6: "Copper sulfate dissolves in water. Then, we add iron metal in the solution. Because iron is a more active metal than copper, it has higher potential for donating electrons. Copper has negative and iron has positive potential values. Therefore, iron has more tendency to form a compound than copper. As a result, it displaces copper." - (Active agent)

Even though more than half of the Undergraduate and Graduate participants acknowledged the displacement of the particles, limited number of students expressed the attraction between the particles. Among the four groups, conceptual mode of *mutual attraction* was mostly expressed by Undergraduate 1 (f=8, 40%) and Undergraduate 4 students (f=6, 30%). Following example demonstrates the explanation of the conceptual mode of *mutual attraction*:

GRP9: "We need a force to pull the electrons of iron. We need an electron movement from iron to copper. [...] There is an electrostatic interaction... Electrons will be pulled towards a direction [towards copper]... Copper has plus two charge here. It pulls the electrons of iron because it has a positive charge." - (Mutual attraction)

While thinking about the reaction process, some participants focused on the displacement of the metals and expressed the conceptual mode of *displacement of aggregates*. Expression of this conceptual mode decreased gradually as the students progressed through chemistry education (95%, 90%, 60%, and 53% for G12, UG1, UG4, and GR groups, respectively). As students progressed through chemistry education, explanatory power of the conceptual modes they expressed about the reaction process increased. Students with higher level of chemistry education expressed that the reaction took place as the interaction of the metals for electron transfer and the interactions of the ions with water molecules took place. Following interview excerpt illustrates a Graduate student's explanations regarding *changes through interactions*:

GRP10: "Copper and sulfate ions are constantly colliding, interacting and separating in the water. They are in a dynamic motion. Iron is present in the water in a solid form. For example, when iron and copper are in a certain proximity, I mean their physical interaction will make this reaction proceed. I guess, when iron and copper attract each other, there will be an electron exchange. [...] When the electron exchange is complete, copper transfers into solid form and iron moves into the solution. As a result of a redox step, now, we are able to dissolve iron in the water." - (Changes through interactions) When thinking about how the single displacement reaction stops, most of the participants stated that this reaction stops when all reactants were consumed or when the formation of copper solid stops. Such explanations were categorized as *when reactants are gone*. To be more specific, 90% of Grade 12 and 95% of Undergraduate 1 students expressed the conceptual mode of *when reactants are gone*. On the other hand, 15% of Undergraduate 4 (f=3) students thought that the reaction stopped when an equilibrium was reached while only one Undergraduate 4 students described a dynamic equilibrium process. Here, it can be seen that the percentage distributions of conceptual modes were almost the same between Grade 12 and Undergraduate 1 students, except one Grade 12 student stated that this reaction would not stop (see Table 4.16). Following interview excerpt illustrates the explanation of this Grade 12 student:

G12P20: "Products of this reaction are iron sulfate and copper in a solid form. Again, there is an equilibrium state here. The substances can not remain like this all the time. I think that some amount of copper will dissolve and turn back into solid form constantly." - (Dynamic equilibrium)

An Undergraduate 4 student explained the dynamic equilibrium process such that:

UG4P11: "I think that we can not say that this reaction stops. As iron reaches its metallic form, copper may switch to its ionic form again to form a salt with sulfate." - (Dynamic equilibrium)

A Graduate student expressed that this reaction would not stop. Following interview excerpt represents this student's explanation:

GRP9: "I think this reaction would not stop. If the reactants are one to one, there is going to be an equilibrium state. [...] I think, electrons will keep traveling between the particles. So, both Fe^{2+} and Cu^{2+} will be present in the solution." - (Dynamic equilibrium)

Acknowledging that this was a redox reaction as well, most of the participants from all groups stated that this reaction happened due to the presence of an *active agent* (e.g., iron has more activity and copper has tendency to receive electrons). Additionally, some participants in Grade 12 group (f=3, 15%) mentioned that the reaction happens due to attractive forces between the particles. Following interview excerpts illustrate the explanations of Grade 12 and Undergraduate 1 students:

G12P2: "[...] Because iron is more active than copper. Therefore, it can reduce copper." - (Active agent) UG1P7: "Copper... Probably it is about copper being a semi-noble metal. It has more tendency to remain in elemental form. [...] We can say that iron donates electrons easier because it is more active." - (Active agent)

It was found that, as the grade level increased, conceptual modes with more sophistication were expressed by small number of students. Such explanations were observed more among the Undergraduate 4 students (see Table 4.16). Examples from Undergraduate 4 and Graduate students' explanations are presented in the following excerpts:

UG4P6: "Electron affinity of copper is higher than iron when copper is in +2 form. I mean, it [electron affinity] is about atoms loving electrons and their urge for having electrons in their orbitals. [...] Copper wants to take the electrons. Therefore, it creates attractive forces. In iron, electrons are present in a cloud form. When copper and iron are in a certain proximity, protons of copper affect the electrons of iron. Therefore, I think, electron transfer takes place." - (Teleological explanations) GRP12: "Here, iron is in the solid form and copper is in ion form. Because

copper is more stable in solid form than iron, copper is in ion form. Decause form. [...] The reaction happens because of stability. I mean copper in metallic form is more stable than metallic form of iron. Copper takes the electrons and transfers into the elemental form due to stability. Therefore, it can remain in lower energy." - (Causal explanations)

When thinking about the single displacement reaction, progression in the level of chemistry education seemed to change participants' explanations regarding properties and interactions affecting the process. The number of students providing expressions regarding this dimension increased as the level of chemistry education increased. As the students moved to Undergraduate 4 and Graduate years, the sophistication of their conceptual modes increased. All Grade 12 and Undergraduate 1 students who provided explanations regarding this dimension expressed the conceptual mode of *central agent*. Following examples illustrate these explanations:

G12P8: "In order to dissolve, substances have to have more activity. Because iron dissolves here, we can say that it has more reactivity." - (Central agent)

UG1P19: "There are two factors forcing this reaction to continue. First, the presence of the ions in the solution. Second, iron's tendency to donate and copper's tendency to receive electrons." - (Central agent)

Following interview excerpts demonstrate Undergraduate 4 and Graduate students' explanations having more explanatory power:

UG4P4: "[...] When we add iron into the solution, Cu^{2+} receives electrons from iron. In other words, electron transfer takes place between iron and copper. Then, iron atoms donating electron become ions and move into the solution while copper atoms receiving electrons turns into the elemental form." - (Multiple agents in sequence)

GRP7: "Considering the tendencies of iron and copper for donating and receiving electrons, their mutual interactions regarding electron transfer make this reaction occur. When Cu^{2+} ions interact with iron atoms, electron transfer takes place." - (Multiple interacting agents)

While thinking about energetic and entropic drivers of the single displacement reaction, very limited number of participants provided explanations. While none of the Grade 12 student provided explanations, all Undergraduate 1 participants who provided answer (f=5) expressed conceptual mode of *energy driving*. Following excerpt demonstrate Undergraduate 1 students' explanations:

UG1P16: "Considering that this reaction is spontaneous, I think that energy of the products decreases as the reaction medium releases heat." - (Energy driving)

The participants from Undergraduate 4 and Graduate groups stated that this reaction was driven by both energetic and entropic factors as it can be seen in the following example:

UG4P17: "Copper's reduction potential is greater than iron's reduction potential. When we calculate the cell potential, it turns out to be positive. This indicates that this reaction is spontaneous. We can say that energy is not supplied to this reaction medium." - (Energy and entropy driving)

Conceptual modes	G12	levels. UG1	UG4	GR
L .	f (%)	f(%)	f(%)	f(%)
How chemical reactions start				
Active agent	14(70)	12(60)	14 (70)	13(76)
Mutual attraction	4(20)	8 (40)	6(30)	3(18)
No response	2(10)	0 (0)	0 (0)	1(6)
How chemical reactions proceed				
Displacement of aggregates	19 (95)	18 (90)	12 (60)	9(53)
Bonds broken and reformed	0 (0)	0 (0)	0 (0)	1(6)
Changes through interactions	0 (0)	1(5)	7(35)	8 (47)
No response	1(5)	1(5)	1(5)	0 (0)
When chemical reactions stop				
When reactants are gone	18 (90)	19 (95)	16 (80)	15(88)
Stops at equilibrium	1(5)	1(5)	3(15)	1(6)
Dynamic equilibrium	1 (5)	0 (0)	1(5)	1(6)
No response	0 (0)	0 (0)	0 (0)	0 (0)
Why chemical reactions happen				
Active agent	16 (80)	18 (90)	18 (90)	14(82)
Attractive forces	3(15)	0 (0)	1(5)	1(6)
Teleological explanations	1 (5)	0 (0)	3(15)	1(6)
Causal explanations	0 (0)	0 (0)	1 (5)	1(6)
No response	0 (0)	2(10)	0 (0)	0 (0)
What causes chemical reactions				
Central agent	4(20)	8 (40)	7(35)	11(64)
Multiple agents in sequence	0 (0)	0 (0)	3(15)	3(18)
Multiple interacting agents	0 (0)	0 (0)	2(10)	2(12)
No response	16 (80)	12~(60)	8 (40)	1(6)
What drives chemical reactions				
Energy driving	0 (0)	5(25)	0 (0)	0 (0)
Energy and entropy driving	0 (0)	0 (0)	1(5)	1(6)
No response	20(100)	15 (75)	19 (95)	16 (94)

 Table 4.16. Frequencies of conceptual modes regarding the single displacement reaction across different grade levels.

It is important to note that more Undergraduate 1 participants provided explanations regarding this dimension than Undergraduate 4 and Graduate participants.

4.2.3. Decomposition Reaction

As a representative of decomposition reactions, the participants were given decomposition of calcium carbonate ($CaCO_3$). Particles of all substances are in constant motion. When particles have enough energy to overcome the intermolecular forces due to the vigorous motion, a chemical reaction takes place and products are formed. In this case, an increase in temperature of the medium results in an increase in the kinetic energy of particles. Increasing in the kinetic energy causes bond breaking, and consequently, a decomposition reaction takes place to produce CaO (s) and CO_2 (g). Due to the structure of CO_3^{2-} ion, there are three oxygen particles having valence electrons. These electrons are delocalized. Given the energy of the system, constant vibration of the particles, and the presence of Ca^{2+} ion, there is a probability of transferring these valence electrons to an oxygen particle to produce O^{2-} ion; consequently, this results in the formation of CO_2 in the gas form. Given Ca^{2+} and O^{2-} ions in the medium, strong electrostatic interactions between them leads to the formation of CaO ionic lattice. The reaction is entropically driven because of the dramatic increase in entropy as a result of $CO_2(g)$ formation. In gas phase, particles have more orientations available in which they can be arranged due to the higher kinetic energy of the particles and the increase in the volume occupied. Due to the requirement of energy for breaking C–O bonds, the reaction is endothermic and is favorable in high temperatures.

Frequencies and percentages of classification categories in participants' expressions were given in Table 4.17. Almost all students from all groups classified this reaction as a *decomposition* reaction. Only 2 students (10%) from Grade 12 group did not express any classification category for this reaction. This was given in the *other* category in Table 4.17.

Data analysis showed that the dimensions how chemical reactions proceed, why chemical reactions happen, what causes chemical reactions, and what drives chemical *reactions* seemed to depend on the level of chemistry education for the decomposition reaction. Conceptual modes emerged for the decomposition reaction were given in Table 4.18.

Classification categories	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
Decomposition	18 (90)	20 (100)	20 (100)	17 (100)
Other	2(10)	0 (0)	0 (0)	0 (0)
Total	20 (100)	20 (100)	20 (100)	17(100)

 Table 4.17. Frequencies of classification categories regarding decomposition reaction across different grade levels.

When thinking about how the decomposition reaction started, all participants stated that *external forces* started the reaction. In this case, the external force was heat or another energy source. Even though all participants expressed conceptual mode of *external forces*, students' explanations shifted to descriptions in the particulate level, as the level of chemistry education increased. Following interview excerpts demonstrate students' explanations:

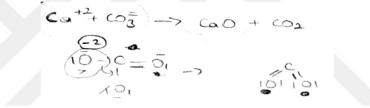
G12P3: "I think this solid took energy and transformed into calcium oxide solid and carbon dioxide gas." - (External forces)
UG1P2: "When necessary amount of energy is supplied, CO₂ separates from the compound. We need a lot of energy to produce a gas. When elements forming CO₂ have enough energy, they speed up and separate from the solid." - (External forces)
UG4P16: "This reaction starts when we supply heat [...] Calcium carbonate molecules will vibrate faster and then, carbon dioxide gas will be produced." - (External forces)
GRP2: "In order to break the bonds, we need to supply energy. It could be heat." - (External forces)

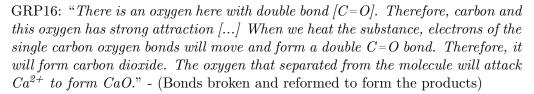
Participants' explanations regarding the process of decomposition reaction revealed that sophistication level of conceptual modes increased as the grade level increased. Almost all participants from Grade 12 group (f=17, 85%) stated that the reaction progressed simply by breaking of calcium carbonate into calcium oxide and carbon dioxide (*decomposition of aggregates*). Following interview excerpt demonstrates an example of Grade 12 participants' explanations:

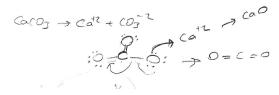
G12P13: "Energy decomposes the compound into other molecules. As a result, gas molecules separate from the solid." - (Decomposition of aggregates)

Following examples show the increase in sophistication of students' conceptual modes (see Table 4.18) :

UG1P3: "When we heat calcium carbonate, one of the oxygens will receive an electron from the bond [C-O bond] to become O^{2-} . Then, it will combine with calcium." - (Bonds broken and reformed to form the products)







When thinking about when would the decomposition reaction stop, the majority of participants' expressions were distributed among the conceptual modes of when reactants are gone and when external force is removed. A very limited number of students from Grade 12 (f=1), Undergraduate 1 (f=1), and Undergraduate 4 (f=2) groups mentioned chemical equilibrium. Following example shows how students expressed the conceptual mode of when external force is removed:

UG4P4: "If we do not supply energy to reach activation barrier, the reaction will stop." - (When external force is removed)

When thinking about why decomposition reaction happened, more than half of the Undergraduate 1 (65%) and Undergraduate 4 (70%) participants and almost half of the Grade 12 (45%) and Graduate (47%) participants expressed conceptual mode of *external forces* (see Table 4.18). However, students progressed to graduate level, expression of conceptual modes with higher explanatory power increased. It is important to note that expression of the conceptual modes among Grade 12 students lower for this reaction when compared with the other reaction types (i.e., double displacement, single displacement, and combination). Following examples illustrate the expression of various conceptual modes:

UG1P16: "This reaction happened due to heat... Because we supplied heat." - (External forces)

GRP8: "Calcium oxide is more stable. In the structure of carbonate, there is an electron circulation... Resonance... Resonance is not a stable state. Therefore, calcium oxide is more stable. It [calcium oxide] has a simpler structure... When structure of a molecule is too complex [carbonate], it gets unstable." - (Causal explanations)

When thinking about the factors or the properties affecting the decomposition reaction, all Grade 12 participants that provided explanations regarding *what causes chemical reactions* (f=11, 55%) stated that the reaction was affected by a central agent. In this case, the central agent under consideration was heat. Explanations of Grade 12 students can be seen in the following example:

G12P9: "This is an endothermic reaction. I can continue as long as we keep supplying heat to the reaction medium. Otherwise, the reverse reaction will happen." - (Central agent)

Explaining the conceptual mode of *multiple agents in sequence* increased as students progressed through chemistry education. Following interview excerpt demonstrates their explanation of this conceptual mode:

UG4P4: "When we start heating, carbon-oxygen bond in carbonate molecules will break. Bond electrons will travel to the oxygen atom to form O^{2-} . Then, O^{2-} and Ca^{2+} will attract each other and form ionic bond. On the other hand, after the oxygen separates from carbonate, carbon will become a carbocation. It will

form another double bond with the electrons of the oxygens and consequently will produce carbon dioxide." - (Multiple agents in sequence)

Conceptual modes	G12	UG1	UG4	GR
	f~(%)	f (%)	f (%)	f~(%)
How chemical reactions start				
External forces	20 (100)	20 (100)	20 (100)	17(100)
No response	0 (0)	0 (0)	0 (0)	0 (0)
How chemical reactions proceed				
Decomposition of aggregates	17 (85)	8 (40)	9(45)	3(18)
Bonds broken and reformed	1(5)	12(60)	10(50)	14(82)
No response	2(10)	0 (0)	1(5)	0 (0)
When chemical reactions stop				
When reactants are gone	19 (95)	18 (90)	13 (65)	17(100)
When external force is removed	10 (50)	13 (65)	10 (50)	13 (76)
Stops at equilibrium	0 (0)	1(5)	2(10)	0 (0)
Dynamic equilibrium	1(5)	0 (0)	0 (0)	0 (0)
No response	0 (0)	0 (0)	0 (0)	0 (0)
Why chemical reactions happen				
External forces	9(45)	13 (65)	14(70)	8 (47)
Attractive forces	0 (0)	1(5)	1(5)	0 (0)
Teleological explanations	1 (5)	1(5)	1(5)	1(6)
Causal explanations	2(10)	1(5)	2(10)	5(29)
No response	8 (40)	4 (20)	2(10)	3(18)
What causes chemical reactions				
Central agent	11 (55)	7(35)	6(30)	8 (47)
Multiple agents in sequence	0 (0)	1(5)	6(30)	8 (47)
No response	9(45)	12(60)	8 (40)	1(6)
What drives chemical reactions				
Energy driving	0 (0)	1(5)	1(5)	4(24)
Energy-entropy merged	0 (0)	2(10)	2(10)	3(18)
Energy and entropy driving	0 (0)	1(5)	3(15)	5(29)
No response	20 (100)	16 (80)	14(70)	5(29)

 Table 4.18. Frequencies of conceptual modes regarding decomposition reaction across

 different grade levels.

When thinking about energetic and entropic factors driving the decomposition reaction, none of the Grade 12 students provided explanations. Following the Grade 12 students, very few Undergraduate 1 students expressed their conceptual modes regarding *what drives chemical reactions*. It can be concluded that as the grade level increased, the frequency of explanations regarding the dimension *what drives chemical reactions* increased. In the Graduate group, 4 of 17 participants stated that the reaction was driven by energetic factors as shown in the example:

GRP11: "Under normal conditions, this reaction does not happen spontaneously. It happens only when we supply heat to provide necessary energy [...] When I think about the crystal structure of calcium oxide, I expect it to be more close packed. A structure including two atoms is stronger than a structure including one atom and one compound. Therefore, probably, calcium oxide is more stable than the reactant. It might prefer to transform into this [calcium oxide], in order to have a more stable form." - (Energy driving)

On the other hand, 2 of 20 Undergraduate 1 students, 2 of 20 Undergraduate 4 students, and 3 of 17 of Graduate students used energy and entropy terms interchangeably or had alternative conceptions. Such explanations can be seen in the following interview excerpt:

UG4P10: "This reaction is not favorable. When I consider delta G... I don't know... Because we supply heat to the reaction medium, it is not favorable. Calcium carbonate is a stable molecule. However, we make it less stable with heat. I can say that energy of the products decreases because, I force a very stable molecule to decompose into less stable two molecules. Carbon dioxide is a gas... So, it is unstable." - (Energy-entropy merged)

3 of 20 Undergraduate 4 students, 5 of 17 Graduate students, and 1 of 20 Undergraduate 1 students stated that this reaction was driven by both energetic and entropic factors. Following example illustrates students' explanations regarding the conceptual mode of energy and entropy driving:

GRP13: "Chemical reactions favor disorder. So we should consider entropic factors in this reaction because a substance transforms into a gas, a structure with disorder. On the other hand, we supply energy to break the bonds. Enthalpy is dominant here as well. Because the presence of a gas in the products is not enough to drive a chemical reaction." - (Energy and entropy driving)

4.2.4. Combination Reaction

As a combination reaction, the participants were given the combustion reaction of magnesium metal (Mg) producing MgO (s) and O_2 (g). Due to the transfer of electron between Mg and O_2 , this reaction can be classified as a redox reaction as well. Particles of chemical substances are in constant motion to collide. When they collide with proper orientation and kinetic energy, the particles reach the activation energy to form the products. An increase in the energy of reaction medium increases the possibility of reaching the activation energy. Random collisions of magnesium metal and oxygen gas leads to the transfer of electron between the substances. Electron transfer takes place from magnesium to oxygen leads to formation of Mg^{2+} and O^{2-} . Given the positive and negative ions in the reaction medium, strong interactions between them leads to formation of MgO ionic lattice. MgO has lower energy than the reactants, so that there is a large amount of energy release during the reaction which is an exothermic process. Due to the large amount of energy release, the entropy change of the surrounding (ΔS_{surr}) overcomes the entropy change of the system (ΔS_{sys}) . Consequently, entropy change of the universe (ΔS_{univ}) indicates an increase in the entropy of the universe, which satisfies the second law of thermodynamics.

Frequencies and percentages of classification categories in participants' expressions were given in Table 4.19. The majority of Grade 12 students expressed that this was an either *combination* or *combustion* reaction. Only 20% of Grade 12 students expressed that this was a *redox* reaction while taking either combustion or combination into account. Majority of Undergraduate 1 students thought that this was a *combustion and redox* or *combination*, *combustion*, *and redox* reaction. This pattern was similar within the Undergraduate 4 group but, 20% of graduate participants also thought that this was a *combination reaction*. Graduate participants mostly expressed that this was a *combination* or *redox* reaction.

Data analysis showed that the dimensions how chemical reactions start, how chemical reactions proceed, why chemical reactions happen, what causes chemical reactions, and what drives chemical reactions seemed to depend on the level of chemistry education for the combination reaction. Conceptual modes emerged for the combination reaction were given in Table 4.20.

Classification categories	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
Combination	6 (30)	3(15)	4 (20)	6(35)
Combustion	6 (30)	0 (0)	2(10)	0(0)
Redox	0 (0)	0 (0)	0 (0)	6(35)
Combination and redox	2(10)	0 (0)	3(15)	2(12)
Combustion and redox	2(10)	6 (30)	5(25)	0 (0)
Combination and combustion	0 (0)	3(15)	0 (0)	0 (0)
Combination, combustion, and redox	0 (0)	6 (30)	4 (20)	0 (0)
Other	4 (20)	2(10)	2(10)	3(18)
Total	20 (100)	20 (100)	20 (100)	17(100)

Table 4.19. Frequency of classification categories regarding combination reaction across different grade levels.

When thinking about how the combination reaction started, almost all participants stated that either an *active agent* (e.g., oxygen) or *external forces* (e.g., heat) started the reaction. Between these two conceptual modes, the majority of the participants expressed the conceptual mode of *external forces*. Only 3 of 20 Undergraduate 4 students expressed that the reaction started due to *random collisions* of the particles. Expressions of the conceptual modes regarding *how chemical reactions start* can be seen in the following examples:

UG4P9: "[...] There is going to be electron transfer. Because oxygen is in gas form, it is disordered. Magnesium is more stable. Probably it starts due to oxygen because it has more mobility." - (Active agent) UG1P9: "How it starts... Should I start with burning magnesium with a match [...] It starts similar with how we burn a piece of paper." - (External forces) UG4P18: "It starts with collision of gas particles with the solid. Gas particles constantly collide with the solid. I think it starts like this." - (Random collisions) When explaining the reaction process, more than half of the Grade 12, Undergraduate 1, and Undergraduate 4 participants considered oxygen and magnesium as aggregates and expressed the reaction process as the combination of these particles (see Table 4.20). As the grade level increases, students tended to describe electron transfer among the particles and their interactions by expressing the conceptual mode of *changes through interactions*. This conceptual mode was expressed more by the Graduate (47%) students. Distribution of the conceptual modes among Grade 12 and Undergraduate 4 students was similar. Undergraduate 1 students, on the other hand, expressed the conceptual mode of *combination of aggregates* less frequently than Grade 12 and Undergraduate 4 students. They focused on the conceptual mode of *bonds broken and reformed* more than these groups, and they expressed the conceptual mode of *changes through interactions* less frequently than these groups. It can be concluded that among all grade levels, students from the Graduate group tended to express the conceptual modes with higher explanatory powers than the other students. Students' explanations regarding the reaction process can be seen in the following examples:

G12P3: "When we burn magnesium, it combines with oxygens and and produce magnesium oxide." - (Combination of aggregates)

UG1P9: "When we heat the reaction medium, magnesium and oxygen simultaneously become plus and minus two charged ions. Magnesium oxide is produced at the surface of the magnesium interacting with oxygen. So, when we turn these atoms into ions, they can not remain without a reaction. They form a compound." - (Bonds broken and reformed to form the products)

GRP16: "[...] Here, magnesium donates electrons to oxygen. Magnesium has metallic bonds and their electrons are moving freely. Therefore, it can easily donate electrons. When we supply energy, we increase orbital energies to the upper levels. It makes easier to donate electrons. There are oxygen atoms ready to receive these electrons. Oxygen receives the electrons. So, it does not need to have double covalent bonds anymore. It will form magnesium oxide. The other oxygen will interact with magnesium particles similarly. As a result, we will have two magnesium oxides." - (Changes through interactions)

When thinking about how the combination reaction stop, all participants mentioned when reactants are gone and/or when external force is removed. These explanations were similar to the conceptual modes expressed for the decomposition reaction (see Tables 4.18 and 4.20).

Regarding why chemical reactions happen dimension for the combination reaction, participants from Grade 12 (35%) and Undergraduate 1 (75%) groups focused on the conceptual mode external forces by stating that the reaction happened due to the heating of the reaction medium or exposing magnesium directly to flame. On the other hand, as the grade level increased, students' understanding shifted to the particulate view of the causality of the combination reaction. The four of 20 Undergraduate 4 and the three of 17 Graduate students focused on the properties of the particles involved in the reaction process while explaining the reasons behind the reaction. Following excerpts illustrate these explanations:

UG4P4: "When we heat magnesium, electrons jumped to a higher energy state, but it is not favorable. It wants to lower it down. Because of the energy, magnesium can not return its ground state. Therefore, it will prefer attacking the empty orbitals of oxygen. The main reason is to lower its energy. - (Teleological explanations)" GRP17: "The reason is... I think that magnesium oxide has lower energy than

the others. Low energy means a more stable structure. I think this is the reason." - (Causal explanations)

While considering the properties and the agents affecting chemical processes, six of 20 Undergraduate 1 students focused on a *central agent* affecting the reaction process. On the other hand, six of 20 Grade 12 students stated that the reaction process is affected by the interaction of multiple agents in a sequence (i.e., *multiple agents in sequence*). It is important to note that more Grade 12 students expressed a conceptual mode with high explanatory power (i.e., *multiple agents in sequence*) than Undergraduate 1 students. While Undergraduate 4 students focused on the conceptual modes of *central agent* and *multiple interacting agents*, Graduate students mostly expressed the conceptual modes of *central agent* and *multiple agents in sequence*.

different grade levels.				
Conceptual modes	G12	UG1	UG4	GR
	f (%)	f (%)	f (%)	f (%)
How chemical reactions start				
Just happens	1 (5)	0 (0)	0 (0)	0 (0)
Active agent	3(15)	1(5)	6(30)	8 (47)
External forces	14(70)	19 (95)	10(50)	9(53)
Random collisions	0 (0)	0 (0)	3(15)	0 (0)
No response	2(10)	0 (0)	1(5)	0 (0)
How chemical reactions proceed				
Combination of aggregates	13 (65)	11 (55)	$13 \ (65)$	3(18)
Bonds broken and reformed	2(10)	5(25)	2(10)	6(35)
Changes through interactions	5(25)	4(20)	5(25)	8 (47)
No response	0 (0)	0 (0)	0 (0)	0 (0)
When chemical reactions stop				
When reactants are gone	18 (90)	20 (100)	18 (90)	16(94)
When external force is removed	4(20)	3(15)	0 (0)	5(29)
No response	0 (0)	0 (0)	2(10)	0 (0)
Why chemical reactions happen				
Active agent	2(10)	4(20)	5(25)	9(53)
External forces	7(35)	15(75)	3(15)	5(29)
Attractive forces	2(10)	0 (0)	1(5)	0 (0)
Teleological explanations	1(5)	1(5)	3(15)	0 (0)
Causal explanations	2(10)	1(5)	0 (0)	3(18)
Probability	0 (0)	0 (0)	1(5)	0 (0)
No response	6(30)	0 (0)	7(35)	0 (0)
What causes chemical reactions				
Central agent	3(15)	6(30)	5(25)	6(35)
Multiple agents in sequence	6(30)	1(5)	2(10)	9(53)
Multiple interacting agents	0 (0)	0 (0)	3(15)	1(6)
No response	11 (55)	13 (65)	10(50)	1(6)
What drives chemical reactions				
Energy driving	0 (0)	2(10)	3(15)	4(23)
Energy-entropy merged	0 (0)	0 (0)	0 (0)	1(6)
Energy and entropy driving	1 (5)	2(10)	1(5)	2(12)
No response	19 (95)	16(80)	16(80)	10(59)

 Table 4.20. Frequencies of conceptual modes regarding combination reaction across

 different grade levels.

Regarding energetic and entropic drivers of the combination reaction, only one Grade 12 students provided an explanation stating that the reaction was driven by both energetic and entropic factors. Two of 20 Undergraduate 1, three of 20 Undergraduate 4 students, and four of 17 Graduate participants stated that the reaction was driven by energetic factors. Remaining 2 of 20 Undergraduate 1, one of 20 Undergraduate 4, and 2 of 17 Graduate students expressed that the reaction was driven by both energetic and entropic factors.



5. DISCUSSION

The aim of the present study was to map students' conceptual progression of chemical mechanism (How do chemical reactions happen?) and chemical causality (Why do chemical reactions happen?). In order to attain this goal, following research questions guided the study:

- (i) How do students' conceptual modes related to chemical mechanism change across different grade levels?
- (ii) How do students' conceptual modes related to chemical causality change across different grade levels?
- (iii) How do students' conceptual modes related to chemical mechanism and chemical causality change with respect to the type of reaction under analysis?

In order to address these research questions, qualitative data collected from four groups of students, namely, Grade 12 (n=20), Undergraduate 1 (n=20), Undergraduate 4 (n=20), and Graduate (n = 17) through semistructured interviews. Interview protocol included four types of chemical reactions (i.e., double displacement, single displacement, decomposition, and combination) with different driving forces, chemical bonds, and physical states. This cross-sectional research study adopted grounded theory as a research methodology, and the data were analyzed through constant comparative approach (Glaser and Strauss, 1967).

As a result of data analysis, following dimensions emerged for the concepts under investigation (i.e., chemical mechanism and chemical causality):

- (i) Concept: Chemical mechanism (How do chemical reactions happen?)
 - Dimension: How chemical reactions start
 - Dimension: How chemical reactions proceed
 - Dimension: When chemical reactions stop
- (ii) Concept: Chemical causality (Why do chemical reactions happen?)

- Dimension: Why chemical reactions happen
- Dimension: What causes chemical reactions
- Dimension: What drives chemical reactions

Analysis of students' explanations revealed several conceptual modes for each dimension. Conceptual modes reflected students' various descriptions of the dimensions regarding the different types of chemical reactions (Yan and Talanquer, 2015). In order to address the research questions, conceptual modes were sequenced in an increasing explanatory power. However, increasing level of sophistication of the conceptual modes is not linear. It was found that expression of the conceptual modes depended on the type of reaction under analysis and students' level of chemistry education. There were dominantly expressed conceptual modes for some of the dimensions. Conceptual modes emerged for each dimension were represented in Figure 5.1.

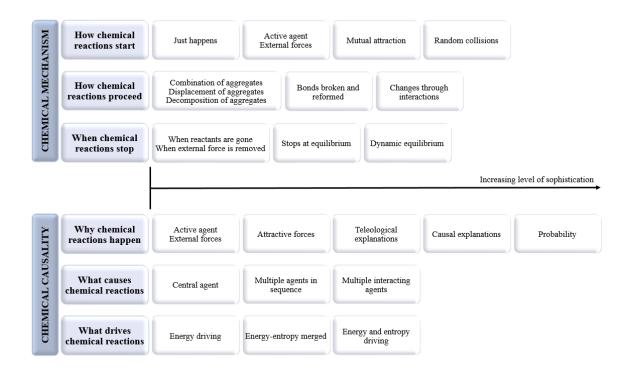


Figure 5.1. Dimensions and conceptual modes regarding chemical mechanism and chemical causality

When overall progression was examined, there observed dramatic changes in the expressions of the conceptual modes from Grade 12 to Graduate level while describing

how chemical reactions proceed, why chemical reactions happen, what causes chemical reactions, and what drives chemical reactions. In other words, students' expressions of the conceptual modes depended on the grade level mostly when describing the reaction process and when explaining chemical causality.

When thinking about how chemical reactions proceed, Grade 12 students tended to describe the reaction processes in terms of *combination/displacement/decomposition* of aggregates with little or no mention of the processes taking place at the molecular level. However, as the grade level increased, the participants started to conceptualize reaction processes as bond breaking and bond formation. Describing chemical processes in terms of simultaneous interactions among various particles was limited among Undergraduate 4 and Graduate participants. These findings were consistent with the findings proposed by Yan and Talanquer (2015). In their study, the researchers also found that advanced undergraduate students tended to describe chemical reactions in terms of bond breaking and bond formation, and only advanced graduate participants explained the reactions in terms of *multiple interacting agents*.

Even though there seems to be an increase in the expressions of the conceptual modes with higher explanatory power regarding the dimension of *why chemical reactions happen* as students move to advanced levels, the progression was less clear. For example, the expression of conceptual mode of *active agent*, which has the less explanatory power, increased as the grade level increased. Furthermore, the conceptual mode of *attractive forces*, which implied that chemical reactions happen due to the electrostatic interactions between the particles, was expressed more by the Grade 12 students. This conceptual mode expressed least by the Graduate students. However, when expressions of the conceptual modes of *teleological explanations*, *causal explanations*, and *probability* were examined, it can be stated that they were expressed mostly by the Undergraduate 4 and Graduate students, who had more progress in chemistry education. Concerning *teleological explanations*, students expressed that the substances wanted or needed to be stable or reach octet. While expressing this conceptual mode, the participants mostly focused on kinetic stability or thermodynamic stability which did not include further explanations. The language that the students used implying that the particles had wants and needs seemed to be adopted by the instructors and textbooks (Talanquer, 2007, 2013). It is not clear that whether the participants really believed that particles have needs and wants and is open to debate whether such expressions have strong explanatory power (Talanguer, 2007, 2013). However, it was claimed that there is no need for such explanations in physical sciences (i.e., physics and chemistry) (Talanquer, 2013). In the sample of this study, such explanations were mostly common among Undergraduate 4 students. When students progressed to Graduate level, their preference for *causal explanations* increased, which indicated that there were not any statements regarding wants and needs of the particles in students' explanations. These findings were similar to the study by Weinrich and Talanquer (2015). They also found that *teleological explanations* were common among the students at intermediate levels (e.g., undergraduate students). On the other hand, they found that *causal explanations* were most common among the Graduate students. Talanquer (2013) found that there was no statistical significant difference among undergraduate and graduate students in terms of preferring teleological explanations over causal explanations. However, there were minor differences depending on the reaction type that the students were presented. Therefore, this issue needs further investigation.

Concerning the particles, external factors, and interactions affecting the chemical reactions, the majority of the participants focused on a *central agent* affecting chemical processes. Depending on the nature of the chemical reaction under analysis, the central agent was either a reactant, or an external factor such as heat or electricity. Grade 12 and Undergraduate 1 students focused on a central agent when thinking about the processes and agents affecting chemical reactions. Expressions of the conceptual modes with higher explanatory power focusing on multiple agents and events were more common among the Undergraduate 4 and the Graduate participants. The conceptual mode of *multiple agents in sequence* was expressed more by the Graduate students. On the other hand, the expression of the conceptual mode of *multiple interacting agents* was more frequent among the Undergraduate 4 students.

When thinking about energetic and entropic factors affecting the chemical reactions, expressions of the conceptual modes were quite low when compared with the other dimensions. However, expressions of the conceptual modes increased as the grade level increased. Only one student from Grade 12 group provided explanations regarding energetic and entropic factors affecting chemical reactions. A total of nine Undergraduate 1 students stated that chemical reactions were driven by energetic factors by comparing the energies of the reactants and products by mentioning energy taken or released by the reaction under analysis. Consistent with the findings from the study by Weinrich and Talanquer (2015), the majority of explanations by the Undergraduate 4 students were distributed among the conceptual modes of *energy driving* and *energy* and entropy driving. Some advanced level students in the current sample considered energy as an internal driver and mentioned enthalpy, bond energies, or structural stability while judging the reactivity of the substances. However, some students from lower grade levels mentioned energy as an external factor driving the reactions. In the current study, students' views included entropic factors as the grade level increased, and a total of 10 Graduate students expressed that the reactions were driven by both energetic and entropic factors by describing their interpretations of Gibbs energy and its equation ($\Delta G = \Delta H - T\Delta S$).

When students' overall progression was examined regarding chemical mechanism and chemical causality, common expressions of the participants were determined and mapped as described above. However, it was also found that students' expressions depended on the reaction type under analysis. For example, when describing how single displacement reaction (which had an electron transfer process) started, the majority of the participants focused on an *active agent* which initiates the reaction. However, when explaining the double displacement reaction, the participants mostly focused on the conceptual mode of *mutual attraction*. All participants in the sample expressed the conceptual mode of *external forces* (e.g., heat) when explaining the initiation of the decomposition reaction and combination reaction. While thinking about the reaction processes, the participants mostly focused on *combination/displacement/decomposition of aggregates* for all reaction types. However, such explanations seemed to decrease as the grade level increased, and the participants with advanced level of chemistry education (i.e., Undergraduate 4 and Graduate levels) expressed the reactions in terms of bond breaking and bond forming and interactions among the particles. Concerning the dimension of when chemical reactions stop, the conceptual modes of stops at equi*librium* and *dynamic equilibrium* were expressed for the double displacement, single displacement, and decomposition reactions. The conceptual mode of dynamic equilibrium was expressed mostly for the double displacement reaction and not expressed for the combination reaction at all. Here, one can interpret that students thought that dynamic equilibrium processes occur mostly in reactions taking place in aqueous media. The conceptual mode of stops at equilibrium was mostly expressed by the Undergraduate 4 students, and the conceptual mode of *dynamic equilibrium* was mostly expressed by the Grade 12 and the Graduate participants. Even though there seems to be an increase in the expression of the conceptual modes with high explanatory power (i.e., stops at equilibrium and dynamic equilibrium), overall expression of these conceptual modes were quite low for all grade levels (see Table 4.6). While explaining why chemical reactions happen, expressions of the conceptual modes highly depended on the reaction type. For example, the conceptual mode of *attractive forces* was mostly expressed for the double displacement reaction. For the single displacement reaction, which included an electron transfer process, the participants frequently expressed the conceptual mode of *active agent*. For the decomposition and the combination reactions, the conceptual mode of *external forces* was mostly expressed. Additionally, graduate students focused on *active agent* for the combination reaction which can be classified as combustion and a redox reaction as well. While expressing the conceptual mode of *causal explanations*, the participants mentioned the stability of the substances. This conceptual mode was mostly expressed for the decomposition reaction, which was an endothermic reaction. Following the decomposition reaction, *causal explanations* were utilized while describing the combination reaction, which was the combustion of magnesium metal (i.e., an exothermic reaction). Students seemed to ground their explanations on stability while considering the reactions having obvious heat absorption or release. It seemed that recognizing heat absorption and heat release triggered students' assumptions regarding the enthalpy of the reactions and stability of the substances. In parallel to these findings Weinrich and Talanquer (2015) suggested that students' conceptual modes depended on the particular features of the reactions under analysis. The features that the students pay attention to depend on their previous experiences and the chemical reactions

under analysis (Weinrich and Talanquer, 2015). While thinking about the particles and interactions affecting chemical processes, the students mentioned *central agent*, which could be the particles with mobility or heat depending on the reaction type, affected the reactions. It was frequently expressed while thinking about single displacement, decomposition, and combination reactions. The participants tended to sequence the agents and the processes as the factors affecting the reactions mostly for decomposition and combination reactions (*multiple agents in sequence*). The conceptual mode of multiple interacting agents was mostly expressed for the double displacement reaction which overlapped with their explanations regarding the reaction process expressed by the conceptual mode of *changes through interactions*. Expression of these conceptual modes, namely, changes though interactions and multiple interacting agents, had the same trend across the grade levels. They were less frequently expressed by the Grade 12 and the Undergraduate 1 students, and such conceptual modes were mostly expressed by the Undergraduate 4 students (see Table 4.14). It was found that the conceptual modes regarding what drives chemical reactions were mostly expressed while thinking about the decomposition (endothermic) and combination (exothermic) reactions. Similar to the expression of the conceptual mode of *causal explanations*, expression of the conceptual modes regarding the dimension of what drives chemical reactions depended on the consideration of heat absorption or release. In other words, evaluating the reactions with respect to their enthalpies seemed to trigger students' assumptions regarding thermodynamic factors.

Findings of the current study suggested that there were differences in students' expressions based on the grade level. The findings suggested that students need to improve their understanding of thermodynamics, collision theory, intermolecular and intramolecular interactions, and chemical kinetics and connect these concepts to provide deeper explanations for chemical processes and chemical causality.

5.1. Implications

The findings of this study provided insights into chemistry education and research in chemistry education. Sevian and Talanquer (2014) suggested that current instructional approaches focus on introducing fundamental chemistry concepts in an isolated way. This claim can be confirmed when the accumulation of the concepts related with chemical reactions were examined as stated in Section 1.1. Current vision of science education suggests mastering of crosscutting disciplinary concepts for deeper understanding of the discipline (Talanquer, 2016). In order to improve chemistry education, Sevian and Talanquer (2014) suggested learning progression revolving around core practices of chemistry. They determined six crosscutting disciplinary concepts that were judged to be fundamental in chemical thinking. These crosscutting disciplinary concepts are:

- Chemical identity
- Structure-property relationships
- Chemical causality
- Chemical mechanism
- Chemical control
- Benefits-costs-risks

The foci of the current study were the concepts of *chemical mechanism* and *chemical causality*. Yan and Talanquer conducted an empirical study in 2015 targeting the same concepts (i.e., *chemical mechanism* and *chemical causality*). The participants of their study included Undergraduate and Graduate students. As a contribution to the study by Yan and Talanquer (2015), the current study offered empirical data which included different reactions in the interview protocol and Grade 12 participants in the sample for validating the hypothetical learning progression that Sevian and Talanquer (2014) proposed. Findings of the current study suggested that from Grade 12 to Graduate level, students demonstrated significant progression in their understanding of *how chemical reactions proceed* and *chemical causality*. It can be deduced that students need a broad span of time to develop their understanding of these dimensions.

In order to deepen students' understanding of crosscutting disciplinary concepts, teachers should create learning environments including authentic and relevant learning tasks. Furthermore, students are needed to be encouraged for integrating fundamental concepts within and between disciplines. In order to achieve this, students need to address the relationships and connections between the concepts explicitly while engaging in scientific inquiry. When current curricula were examined, it can be seen that fundamental chemistry concepts were presented in an isolated way both in high school and undergraduate-graduate levels (e.g., general chemistry and organic chemistry) (MoNE, 2013a). When difficulties in connecting the concepts in the sample of the current study were considered, rearrangement of science and chemistry curricula can be suggested. Curricular arrangements may include determining and focusing on the crosscutting disciplinary concepts that are fundamental to enhance deeper understanding of the chemistry discipline. When crosscutting disciplinary concepts determined by Sevian and Talanquer (2014) were considered, focusing on such concepts may help in integrating fundamental chemistry concepts. For example, when students think about benefits-costs-risks of chemical practices, they also need to realize the consequences of chemical practices for the wellbeing of the society, environment, and economy. In order to do such analysis, students need to be aware of the properties of the substances and the properties of the chemical processes under consideration. The case mentioned in this example requires the ability to associate the concepts within and across disciplines (e.g., chemistry, science, technology, and society). In order to create learning environments addressing such issues, students should be encouraged to pose and answer relevant questions about core chemistry practices, such as evaluating the costs and consequences of choosing a fuel type over the others (Banks et al., 2015). To be able to evaluate the consequences of using a particular fuel type, students need to be aware of the structure-property relationships of the substances under analysis, which requires the mastery of concepts such as chemical bonding. Furthermore, students need to evaluate the combustion reactions that the fuel alternatives will be involved. In order to do so, they need to be aware of the reaction energies and the properties of the products involving the reactions under investigation. As it can be seen from this example, encouraging students to deal with the core practices of chemistry allows them to study several concepts within and across disciplines (Opitz et al., 2017).

Findings of the research suggested that responses of the participants included *tele*ological explanations stating that the substances had wants or needs (e.g., substances want to be stable or want to reach octet) for forming the products. Research suggested that such explanations may stem from the language adopted by the instructors and the textbooks (Talanquer, 2007, 2013). When students adopt such explanations due to instructions and textbooks, they tend to avoid offering causal explanations involving the properties of particles and interactions regarding chemical processes (Talanquer, 2007, 2013). Chemistry teachers need to create learning environments allowing students to evaluate and deepen their expressions for chemical causality by describing the reactions in terms of dynamic interactions and thermodynamic factors instead of relying simple assumptions such as filling the empty orbitals or being stable (Talanquer, 2013).

Data analysis revealed that students' understanding of *chemical mechanism* and chemical causality depends highly on the type of reaction under analysis. Furthermore, their explanations were mostly determined by their familiarity with the reactions. For example, the participants who were familiar with the reaction between magnesium and oxygen expressed the reaction mechanism differently, compared to the ones who thought that the reaction was simply the rusting of magnesium metal. The participants who thought that the reaction was a slow rusting process mentioned that oxygen particles penetrated through the surface of magnesium. Such explanations led them to express the reaction process in terms of *combination of aggregates*. On the other hand, the participants who were familiar with the reaction tended to mention the effects of heating on the electron movements of magnesium. This resulted in the explanations involving the redox step. In order to enhance clarity while assessing students' understanding of chemical reactions, interview protocols may include macroscopic representations of chemical reactions or demonstrations of reactions (e.g., burning of magnesium). Furthermore, utilizing various sources of data while assessing students' understanding, may provide deeper insight regarding students' conceptualizations of chemical processes. Even though students' drawings and detailed explanations of chemical mechanism were utilized in the current study, encouraging them to use dynamic representations (e.g., animations) while expressing chemical mechanism may allow the researchers to analyze students' understanding from a dynamic perspective.

5.2. Limitations of the Study

This study was based on a cross-sectional design, in order to track the progression in students' understanding of chemical mechanism and chemical causality over several years. This design is different from longitudinal studies in which one can track the same group over a time period to investigate the changes in students' understanding as they progress through chemistry education. Cross-sectional design adopted in this study allowed the researcher to collect the data from multiple groups at a single point of time to compare multiple groups for tracking the changes (Creswell, 2012). Even though, cross-sectional designs are less time consuming and prevent losing participants over a long period of time, it was suggested to perform longitudinal studies which include aligned curriculum, instruction, and assessment practices to validate the proposed hypothetical learning progressions (Duncan, 2009).

In order to obtain variety in the sample (e.g., gender and achievement), Grade 12 participants were recruited from various high schools which included students with several achievements and educational background. However, shy and hesitant participants do not express their ideas in detail (Creswell, 2013). In order to prevent these difficulties that the shy participants would create during the interviews, chemistry teachers were asked to select students that are willing to share their ideas. Therefore, the selection of Grade 12 students based on their teachers' conception of "talkative students", which resulted in the selection of the high achievers of the schools. Average achievements of the high schools that the Grade 12 participants were recruited from were diverse, so that the researcher tried to control this limitation to some extent. Undergraduate and Graduate participants were recruited from a public research university located in Istanbul. The university, that the Undergraduate and the Graduate participants were recruited from, accepted extremely high achieving students according to their scores on a central university entrance exam. Therefore, it can be interpreted that the Undergraduate and the Graduate participants were above average when compared with other Undergraduate and Graduate students in terms of their academic achievement in the context of Turkey. This reduced the representativeness of the participant groups.

In order to ensure that the Grade 12 students were familiar with the reactions in the interview protocol, common representative reactions were selected for each type (i.e., double displacement, single displacement, decomposition, and combination reactions). For each type, one chemical reaction was selected. However, in order to ensure that the students had consistent views within the same reaction type, choosing more than one reaction would have been beneficial. However, this would have resulted in a significant increase in the interview durations, probably giving rise to withdrawals from the study.

Data analysis was performed by utilizing constant comparative approach. Furthermore, coding process were performed with another researcher to ensure that the same meaning was driven from the pieces of data. Especially Grade 12 students' explanations included fragmented and disorganized statements. Thinking out loud allowed them to express their ideas clearly as the interview progressed, but having inconsistent views for a particular chemical process made the coding process and interpretation of the statements difficult when compared with the other groups of students. Even though the interview protocol encouraged the students express their ideas in depth with its semistructured nature, what the researchers interpreted was students' descriptions of the chemical processes, not what they actually had in their minds. How much the researcher reached the students' minds depended on the motivation of the students to express their thoughts deeply and quality of the communication between the researcher and the participants (Berg, 2001).

5.3. Suggestions for Further Research

When the implications and the limitations given in the previous paragraphs were considered, the current study can provide basis for future studies. In order to provide a picture of students' conceptual progressions of chemical mechanism and chemical causality, the current study adopted a cross-sectional design. The current study provided a basis for designing instructional practices which took students' common reasoning patterns into consideration. Such studies may include curricular arrangements focusing on the crosscutting disciplinary concepts which integrate various fundamental chemistry concepts. While designing curricula and instruction, findings of this research may help in aligning curriculum, instruction, assessment tools, and how students already conceptualized chemical mechanism, chemical causality, and related fundamental chemistry concepts, such as chemical bond, energy, entropy, enthalpy. As suggested by the literature, introducing these concepts via traditional lectures which included a series of fragmented concepts is no different from the current instructional approaches (Sevian and Talanquer, 2014). Therefore, students need to be provided relevant and authentic learning tasks which allow them to explicitly address these concepts and the relationships among them while engaging in scientific inquiry and core chemistry practices (Sevian and Talanquer, 2014). These longitudinal studies would also allow the researchers to uncover how students' thinking progress when they are facilitated with targeted, relevant instructional interventions.

In order to adjust the interview duration and ensure the familiarity of the reactions to the Grade 12 students, one representative reaction was chosen for each type (i.e., double displacement, single displacement, decomposition, and combination) in the current study. In a future longitudinal study, it would be beneficial to increase the type of reactions (e.g., organic reactions). Involving more chemical reactions to the assessment tools, curricula, and instructional interventions increases the contexts in which the concepts of chemical mechanism and chemical causality are introduced to the students. By doing so, chemistry teachers and researchers may allow students to generate a universal understanding of how chemical reactions take place and why chemical reactions happen.

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APPENDIX A: PERMISSION LETTERS

In this section, permission letters obtained from directorates of National Education and Institutional Review Board for Research with Human Subjects (İNAREK) were presented.





T.C. SARIYER KAYMAKAMLIĞI İlçe Milli Eğitim Müdürlüğü

Sayı : 74929039-821.01-E.4170242 Konu : Araştırma İzni

28.03.2017

BOĞAZİÇİ ÜNİVERSİTESİ REKTÖRLÜĞÜNE (Eğitim Fakültesi Matematik ve Fen Bilimleri Eğitimi Bölümü Başkanlığı)

İlgi: a) 19.01.2017 tarih ve 93963947/9 sayılı yazısı. b) Kaymakamlık Makamının 27.03.2017 tarih ve 4084542 sayılı Onayı.

İlgi yazınız ile, Matematik ve Fen Bilimleri Eğitimi Bölümü Öğretim Üyesi Doç, Dr. Emine ADADAN ve aynı bölümde Yüksek Lisans öğrencisi olan Merve Nur YAVUZKAYA tarafından, İlçemiz Rotary 100, Yıl Anadolu Lisesi ve Mustafa Kemal Anadolu Lisesi 12. sınıf öğrencilerins yönelik "Lise Öğrencilerinin Kimyasal Reaksiyonlarla İlgili Kavramsal Anlamlarının Değerlendirilmesi" konulu araştırma çalışması yapına isteğinin uygun görüldüğüne dair Kaymakamlık Makamının ilgi (b) Onayı ekte gönderilmiştir.

Bilgilerinizi ve ilgi (b) Onay doğrultusunda gereğini arz ederim.

۰.

İbrahim TAHMAZ İlçe Milli Eğitim Müdürü

Ek: İlgi (b) Onay (1 Sayfa)

Belaliman Mahalini Ceyr Cad. No.5 Sanyar/STANBUL Tel: 0212 229 41 77-78 (Dehilt 126) Fex:0212 229 41 79 E-Portaneniyer/46@meh.gov.tr Internet Advail/http://www.sorgu.meb.gov.tr Stateji Geliptime B680m8 Do evenk gövenli elektronik inne ile imminantete. bitp://www.sorgu.meb.gov.tr detminden 2693-ebd2-3696-934b-2d11 kodo ile teyt: edilebilir.

Figure A.1. Permission letter obtained from Directorate of National Education of

Sariyer district



T.C. SARIYER KAYMAKAMLIĞI İlçe Milli Eğitim Müdürlüğü

Sayı : 74929039-821.01-E.4084542 Konu : Araştırma İzni (Boğaziçi Üniversitesi) 27/03/2017

KAYMAKAMLIK MAKAMINA

İlgi: Boğaziçi Üniversitesi Eğitim Faktiltesinin 19.01.2017 tarih ve 93963947/9 sayılı yazısı.

Boğaziçi Üniversitesi Eğitim Fakültesi İlgi yazıları ile; Matematik ve Fen Bilimleri Eğitimi Bölümü Öğretim Üyesi Doç. Dr. Emine ADADAN ve aynı bölümde Yüksek Lisans öğrencisi olan Merve Nur YAVUZKAYA tarafından İlçemiz Rotary Anadolu lisesi ve Mustafa Kemal Anadolu Lisesi 12. Sınıf öğrencilerine yönelik "Lise Öğrencilerinin Kimyasal Reaksiyonlarla İlgili Kavramsal Anlamlarının Değerlendirilmesi" konulu araştırma çalışması yapma isteğini bildirmiştir.

Söz konusu çalışmanın Türk Milli Eğitiminin genel amaçlarına uygun olarak, ilgili yasal düzenlemelerde belirtilen ilke, esas ve amaçlara aykırılık teşkil etmeyecek şekilde, gönüllülük esasına göre, okul müdürlüğünün denetim ve sorumluluğunda uygulanması şartı ile Müdürlüğümüzce uygun görülmektedir.

Makamlarızca da uygun görülmesi halinde olurlarınıza arz ederim.

İbrahim TAHMAZ İlçe Milli Eğitim Müdürü

Ek: flgi Yazı ve Ekleri (18 Sayfa)

OLUR 27/03/2017

Gürsoy Osman BİLGİN Kaymakam

Balaliman Mahalini Çaye Cad. No:5 Sanyor@TANBUL Tel: 0212 229 41 77-78 (Dabli:120) Fac:0212 229 41 79	Bilgi için : H.PEKTAŞ
E-Posta zariyer14@rash.gov.tr Internet Advesi http://wriyer.meb.gov.tr	Strateji Osliptirze Bollenii
The struck offered addressed increasing increasing the discretion of the structure of the s	training 4c07-097a-3123-938c-1923 kode ils trait editebilis

Figure A.2. Permission letter obtained from Directorate of National Education of

Sariyer district - Continued



T.C. BEŞİKTAŞ KAYMAKAMLIĞI İlçe Milli Eğitim Müdürlüğü

Sayı : 72726603-821.01-E.276904 Konu : Araştırma İzni (Boğaziçi Üniversitesi) 06/01/2017

KAYMAKAMLIK MAKAMINA BEŞİKTAŞ

İlgi:a)Millî Eğitim Bakanlığına Bağlı Okul ve Kurumlarda Yapılacak Araştırma ve Araştırma Desteğine Yönelik İzin ve Uygulama Yönergesi.

b)Boğaziçi Üniversitesi Eğitim Fakültesinin 26/12/2016 tarihli ve 46640510/80 sayılı yazısı.

Boğaziçi Üniversitesi Eğitim Fakültesi ilgi yazıları ile; Matematik ve Fen Bilimleri Eğitimi Bölümü Öğretim Üyesi Doç. Dr. Emine ADADAN ve aynı bölümde Yüksek Lisans öğrencisi olan Merve Nur YAVUZKAYA tarafından ilçemize bağlı Atatürk Anadolu Lisesi, Beşiktaş Anadolu Lisesi, Sakıp Sabancı Anadolu Lisesi ve Kabataş Erkek Lisesinde bulunan öğrencilere yönelik olarak "Lise Öğrencilerinin Kimyasal Reaksiyonlarla İlgili Kavramsal Anlamlarının Değerlendirilmesi" konulu araştırma çalışması yapma isteğini bildirmiştir.

Adı geçen ortaöğretim kurumlarında bulunan öğrencilere yönelik araştırma uygulanmasının yapılması Müdürlüğümüz ilçe inceleme/değerlendirme kurulu tarafından değerlendirilmiş olup, araştırma Müdürlüğümüzce uygun görülmektedir.

Makamlarınızca da uygun görüldüğü takdirde Olurlarınıza arz ederim.

Dr. Önder ARPACI İlçe Milli Eğitim Müdürü

OLUR 06/01/2017

Dr. Abdullah KALKAN Beşiktaş Kaymakamı

Beşikaş Üçe Millî Eğitin Müdürlüğü (Strateji Geliştirme Belümü) Adets: Adaan Saygun Cad.M.Sailî Rûştî Bey Sok.2 Ulus Beşiktaş/İSTANBUL Posta Kodu: 34340 Tel-Pas(Saviral) : (0 212) 325 49 28 Dubřii - 150 Bilgi için: S.SULAK

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Figure A.3. Permission letter obtained from Directorate of National Education of

Beşiktaş district



T.C. BOĞAZİÇİ ÜNİVERSİTESİ İnsan Araştırmaları Kurumsal Değerlendirme Kurulu (İNAREK)

21.12.2016

Doç. Dr. Emine Adadan Boğaziçi Üniversitesi, Eğitim Fakültesi, Matematik ve Fen Bilimleri Eğitimi Bölümü 34342 Bebek / İstanbul emine.adadan@boun.edu.tr

Sayın Araştırmacı,

"Farklı Yaş Gruplarındaki Öğrencilerin Kimyasal Reaksiyonlarla İlgili Kavramsal Gelişimleri" başlıklı projeniz ile yaptığınız Boğaziçi Üniversitesi İnsan Araştırmaları Kurumsal Değerlendirme Kurulu (İNAREK) 2016/78 kayıt numaralı başvuru 21.12.2016 tarihli ve 2016/11 sayılı kurul toplantısında incelenerek etik onay verilmesi uygun bulunmuştur.

Bilgilerinize rica ederim.

Saygılarımızla,

JA Seli>

Doç. Dr. Arzu Çelik Fuss (Başkan) Fen-Edebiyat Fakültesi Moleküler Biyoloji ve Genetik Bölümü Boğaziçi Üniversitesi, İstanbul

Doç. Dr. Öğlem Hesapçı (Üye) İktisadi ve İdari Bilimler Fakültesi İşletme Bölümü Boğaziçi Üniversitesi, İstanbul

Yrd. Doç. Dr. Mine Göl Güven (Üye) Eğitim Fakültesi, İlköğretim Bölümü Boğaziçi Üniversitesi, İstanbul

Yrd. Doç. Dr. Özgür Kocatürk (Üye) Biyo-Medikal Mühendisliği Boğaziçi Üniversitesi, İstanbul

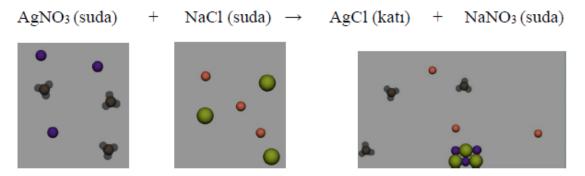
Prof. Dr. Fatoş Gökşen (Üye) Fen Edebiyat Fakültesi Sosyoloji Bölümü Koç Üniversitesi, İstanbul

Figure A.4. Permission letter obtained from Institutional Review Board for Research with Human Subjects (İNAREK)

APPENDIX B: SEMISTRUCTURED INTERVIEW PROTOCOL

Bu görüşmede A + B \rightarrow C + D formundaki kimyasal tepkimeler moleküler gösterimleriyle birlikte verilmiştir. Kimyasal tepkimeler hakkındaki düşüncelerinizi daha iyi anlamak amacıyla size bazı sorular sorulacaktır. Sizden, verilen tepkimeler hakkındaki düşüncelerinizi mümkün olduğunca detaylı bir şekilde ifade etmeniz beklenmektedir.

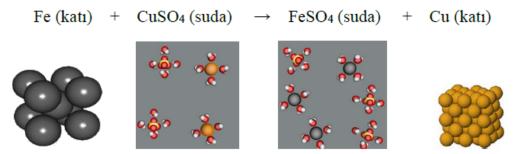
a. Aşağıda gördüğünüz kimyasal tepkimede gümüş nitrat ve sodyum klorür tepkimeye girerek gümüş klorür ve sodyum nitrat oluşturmaktadır. Başka bir deyişle, iki tuz kimyasal tepkimeye girerek iki tuz oluşturmaktadır.



- Görmüş olduğunuz tepkime sizce nasıl başlamıştır?
- Tepkimeye giren maddeleri düşündüğünüzde, tepkimeyi başlatan bir madde olduğunu düşünüyor musunuz? Neden?
- Tepkime sürecini/mekanizmayı çizebilir misiniz? Çizdiğiniz mekanizmayı açıklayınız.
- Görmüş olduğunuz tepkime sizce neden gerçekleşmiştir?
- Görmüş olduğunuz tepkime sizce ne zaman sona ermektedir?

Figure B.1. Semistructured interview protocol - Double displacement reaction

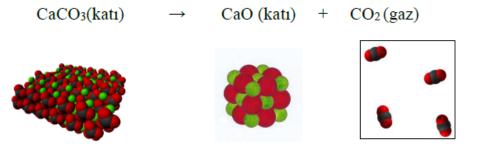
b. Aşağıda gördüğünüz kimyasal reaksiyonda demir katısı ve bakır (II) sülfat tepkimeye girerek demir (II) sülfat ve bakır katısını oluşturmaktadır.



- Görmüş olduğunuz tepkime sizce nasıl başlamıştır?
- Tepkimeye giren maddeleri düşündüğünüzde, tepkimeyi başlatan bir madde olduğunu düşünüyor musunuz? Neden?
- Tepkime sürecini/mekanizmayı çizebilir misiniz? Çizdiğiniz mekanizmayı açıklayınız.
- Görmüş olduğunuz tepkime sizce neden gerçekleşmiştir?
- Görmüş olduğunuz tepkime sizce ne zaman sona ermektedir?

Figure B.2. Semistructured interview protocol - Single displacement reaction

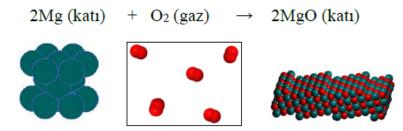
c. Aşağıda gördüğünüz kimyasal reaksiyonda kalsiyum karbonat tepkimeye girerek kalsiyum oksit ve karbon dioksit oluşturmaktadır.



- Görmüş olduğunuz tepkime sizce nasıl başlamıştır?
- Tepkimeye giren maddeleri düşündüğünüzde, tepkimeyi başlatan bir madde olduğunu düşünüyor musunuz? Neden?
- Tepkime sürecini/mekanizmayı çizebilir misiniz? Çizdiğiniz mekanizmayı açıklayınız.
- Görmüş olduğunuz tepkime sizce neden gerçekleşmiştir?
- Görmüş olduğunuz tepkime sizce ne zaman sona ermektedir?

Figure B.3. Semistructured interview protocol - Decomposition reaction

d. Aşağıda gördüğünüz kimyasal reaksiyonda magnezyum katısı oksijen gazı ile tepkimeye girerek magnezyum oksit oluşturmaktadır.



- Görmüş olduğunuz tepkime sizce nasıl başlamıştır?
- Tepkimeye giren maddeleri düşündüğünüzde, tepkimeyi başlatan bir madde olduğunu düşünüyor musunuz? Neden?
- Tepkime sürecini/mekanizmayı çizebilir misiniz? Çizdiğiniz mekanizmayı açıklayınız.
- Görmüş olduğunuz tepkime sizce neden gerçekleşmiştir?
- Görmüş olduğunuz tepkime sizce ne zaman sona ermektedir?

Figure B.4. Semistructured interview protocol - Combination reaction

APPENDIX C: DEMOGRAPHIC FORM FOR GRADE 12 STUDENTS

Demografik Form-Lise Öğrencileri

Ad - Soyad: _			
Cinsiyet:	Erkek 🔲	Kadın 🗌	
Doğum Tarih	i:		
Okul:			
Sınıf:			
Genel Not Or	talaması:		

Kimya dersi notlarınızı dokuzuncu sınıftan itibaren birinci ve ikinci dönem olmak üzere

aşağıda verilen tabloya yazınız.

Sınıf Seviyesi	Birinci Dönem	İkinci Dönem
9. Sinif		
10. Sinif		
11. Sinif		
12. Sınıf		

Figure C.1. Demographic form for Grade 12 students

APPENDIX D: DEMOGRAPHIC FORM FOR CHEMISTRY STUDENTS

Demografik Form-Üniversite Öğrencileri

Ad - Soyad:			
Cinsiyet: E	rkek 🗆 Ka	dın 🗆	
Doğum Tarihi: _			
Okul / Bölüm:			
Smif:		_	
Genel Not Ortala	ması:		
Tamamlanan Kr	edi Sayısı:		
		ini ve harf notlarını şu anda	almakta alduklarınızı
		ini ve nari notarini şu anda	amakta orduktarimizi
ayrıca belirterek			
Dersin Kodu	Harf Notu	Dersin Kodu	Harf Notu
1.		16.	
2.		17.	
3.		18.	
4.		19.	
5.		20.	
6.		21.	
7.		22.	
8.		23.	
9.		24.	
10.			
10.		25.	
11.		25.	

Figure D.1. Demographic form for undergraduate and graduate students

29.

30.

14.

15.