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Cognitive Engagement During Group Learning Activities in Chemistry Courses: An Analysis of Student Discourse

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by

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Abstract

As educators, our goal is to help our students be successful, but in order to accomplish this, we need to understand what factors contribute to student success. One factor, small-group active learning, has been correlated to improved academic outcomes; however, the magnitude of this improvement can vary across different courses, different types of group work, and even across courses that use the same group work structure. Therefore, it is important to understand what aspects of group work contribute to its effectiveness. The work presented in this dissertation investigated one specific aspect: students' cognitive engagement. This was done by analyzing the discourse that occurred between students during group work.

Analysis of the engagement of the group as a whole in General Chemistry suggested some misalignment between how students were expected to engage with activity worksheets and how they actually engaged. Thematic analysis was then used to identify sources of the observed misalignment. The results suggested three themes: 1) model use, where students did not use the models provided in the activity or used them in an incomplete manner; 2) unfamiliar vocabulary, where students engaged at higher modes to understand new scientific terms; and 3) molecular representations, where students struggled to move between different representations of molecules.

Engagement of each individual student within the groups was also analyzed. Results showed trends in engagement related to group size, when the activities were administered during the term, and the type of question being asked during an activity. Students showed higher modes of engagement when groups were small or when students

in larger groups worked together in smaller subsets. They also showed higher modes of engagement as well as less variation in engagement during the second half of the term. In addition, questions which required students to perform calculations had higher modes of engagement than questions that were more conceptual in nature.

Analysis of student group conversations also provided insight into how the activity structure can affect student learning. Using cognitive load theory and the principles of scaffolding, activity worksheets in a Physical Chemistry class were redesigned to break down complex concepts into simpler questions and thereby reduce cognitive overload. Analysis of group conversations and both student and instructor interviews indicated that the redesigned worksheets with scaffolded questions were successful in reducing student struggle and improving student understanding.

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Chapter 1: Introduction

Lecture has been the traditional form of instruction in universities for centuries (Mazer and Hess, 2017). However, in the 1980s, educational performance in the United States was declining due to inadequacies in four main aspects: content, expectations, time, and teaching (National Commission on Excellence in Education, 1983). To address concerns related to teaching, a call to action in 1996 led to a shift from lecture-based teaching to more student-centered pedagogical approaches, i.e., active learning (AL) (National Research Council, 1996). During the past two and a half decades, a wide range of AL approaches have been implemented from methods which target individual participation in the class to methods focused on getting students to work together as a group. In general, a positive relation has been observed between the implementation of active learning methods and student achievement outcomes (Freeman *et al.*, 2014; Wilson and Varma-Nelson, 2016; Deslauriers *et al.*, 2019; Williams *et al.*, 2019). Although this relation is promising, it is not consistent across all AL methods. The magnitude of the improvement varies with both the AL method being implemented and the course it is applied to (Freeman *et al.*, 2014; Rahman and Lewis, 2020).

To understand this variation, it is important to investigate what aspects of active learning contribute to this observed improvement. Research has shown that self-efficacy (students' belief in how well they will do in a course) may explain the positive effect of AL on achievement (Ballen *et al.*, 2017; Corkin *et al.*, 2017). Situational interest (temporary interest stimulated by the task at hand) has also been suggested as a contributing source to the relation between AL and achievement outcomes (Schraw *et al.*, 2001; Corkin *et al.*, 2017). Recent studies have also shown that the implementation of AL classrooms increased student engagement (Odum *et al.*, 2021) and that student engagement positively affected achievement outcomes (Kuh *et al.*, 2008; Delfino, 2019; García-Martínez *et al.*, 2021). Engagement is a complex idea that has multiple dimensions: behavioral, emotional, and cognitive (Fredricks *et al.*, 2004). While student engagement has been defined as the time and energy students commit to their studies (Kuh *et al.*, 2008; García-Martínez *et al.*, 2021), the specific dimensions are defined slightly differently. Behavioral engagement involves participation in academic and social activities, emotional engagement looks at students' positive and negative reactions to classmates and teachers, and cognitive engagement looks at students' effort to comprehend and master new ideas (Fredricks *et al.*, 2004). Previous studies have investigated student engagement as a whole as well as the behavioral and emotional dimensions individually; however, there is limited work studying how students cognitively engage in higher education. Understanding what causes students to cognitively engage at different levels while participating in AL activities could help identify potential sources of the variation in achievement outcomes observed during AL implementation (Freeman *et al.*, 2014; Rahman and Lewis, 2020). This knowledge could also inform the design of future activities so that students can engage more effectively and enhance their understanding of the material presented.

The research presented in this dissertation investigated the different levels students cognitively engage at while participating in small group AL activities during chemistry classes. This work included examining the engagement of the group as a whole as well as the engagement of the individual. Engagement was also examined based on the type of question students were asked. In addition, activity worksheets were modified based on analysis of group conversations.

Statement of Problem

A well-known meta-analysis investigating the effect of AL in science, technology, engineering, and mathematics (STEM) classes on achievement outcomes demonstrated that the use of AL resulted in higher learning gains among students (Freeman *et al.*, 2014); however, the magnitude of these gains varied widely across different STEM subjects. In addition, these gains were significantly larger in under-represented populations (Haak *et al.*, 2011). Since AL is broadly defined and encompasses many different techniques, it is difficult to pinpoint the specific aspects of AL which result in the observed learning gains.

AL methods that involve students working together in small groups are beneficial because they allow students to solve higher order level problems and form more complex responses (Haak *et al.*, 2011; Cooper *et al.*, 2021). However, the effect on achievement outcomes still varied in chemistry classes both across different AL methods which implemented group work and within an individual method (Rahman and Lewis, 2020). Understanding the causes of this observed variation could aid in the implementation of more effective AL strategies which use group work.

In general, achievement outcomes are higher on questions where students were asked to perform a calculation or use a pre-determined set of procedures compared to questions that were more conceptual in nature (Nurrenbern and Pickering, 1987; Pickering, 1990; Sawrey, 1990; Nakhleh, 1993; Zoller *et al.*, 2002; Cracolice *et al.*, 2008;

Surif *et al.*, 2014). However, research has shown that calculation-based questions promoted lower-order thinking skills while conceptual questions promoted higher-order thinking (Zoller *et al.*, 2002). It is possible that the variation observed in student achievement outcomes with AL may be related to the level of engagement students demonstrate while working on different question types. Additionally, the structure of the activity being implemented may affect students' engagement and their understanding of the material being presented. Therefore, understanding how the structure of the activity affects students' mastery of the concepts being introduced may inform possible improvements to these activities.

The degree to which students engage with both the material and with their group members to understand the concepts being taught (i.e., cognitive engagement) could help explain the observed variation in the relation between AL and achievement outcomes. In addition, understanding how engagement changes based on question type could provide insight into possible reasons behind this variation in the effect of AL on achievement outcomes. Therefore, understanding how students engage, both with other group members and with the activity, to comprehend the material can aid in improving how future small group AL environments are implemented. This could reduce the variability currently observed in the effectiveness of AL.

Purpose of Study

In order to reduce differences in the effectiveness of small group AL as measured by achievement outcomes, one first needs to understand what is occurring during small group interactions. This can be done by analyzing the conversations that occur between students while working together on an activity. Multiple studies have examined group conversations through the lens of argumentation or reasoning (Kulatunga *et al.*, 2013; Young and Talanquer, 2013; Becker *et al.*, 2015; Moon *et al.*, 2016); a similar analysis through the lens of engagement could provide insight into how the level of cognitive engagement differs among students and what factors may be contributing to those differences.

The Interactive-Constructive-Active-Passive (ICAP) framework is a theoretical framework which evaluates students' cognitive engagement based on observable behaviors. ICAP can be applied to student conversations to determine the level of cognitive engagement that occurs. This project used ICAP to identify the different levels of cognitive engagement that occur during group work for 1) the group as a whole and 2) for individual students within the group. Differences in expected and observed cognitive engagement level of students during small-group activities were analyzed, and potential factors that may contribute to these differences were identified. Relations between the types of questions being asked and the engagement of the individual were also investigated. ICAP claims that the highest mode of engagement occurs with discourse; therefore, items in activity worksheets were analyzed and modified to improve student discourse.

Research Questions

The overall goal of this project was to examine how students cognitively engage during small-group activities in chemistry courses. The effect of activity design on cognitive engagement was investigated as well as cognitive engagement at the group and individual level. The objectives of this project were addressed by the following research questions:

RQ 1. a) How do student groups' expected and observed cognitive engagement align while participating in small-group active learning activities in chemistry courses?

b) What themes may contribute to any observed misalignment?

RQ 2. a) How does individual students' cognitive engagement vary while participating in small-group active learning activities in chemistry courses?

b) What factors may affect individual students' cognitive engagement?

RQ 3. What relations are observed between the type of question asked in the activities and students' level of cognitive engagement?

RQ 4. a) How can analysis of group conversations inform improvements to learning activities to enhance student understanding?

b) What improvements can be made to learning activities to enhance student understanding?

Significance of Study

This research contributes to current work studying AL by investigating the different levels students cognitively engage at when working in groups. By examining both the content of students' conversation and the manner by which they communicate with one another, the results of this research can aid in understanding: 1) the possible reasons behind the effectiveness of group AL methods and 2) potential sources of the variations in the learning outcomes of students who participate in group AL activities. The results of this research can be used to inform both activity design and the implementation of the activity during group work so that the benefits of small group activities on academic performance become more consistent across all students.

Limitations

Data collection and analysis for this project involved observing conversations between a small number of students at a single institution. Since students must choose to consent to be observed, the sample may not be representative of all students, and therefore, the results are not generalizable to all populations. This study used the ICAP framework to evaluate the level of cognitive engagement based on observable behaviors. Therefore, there is an inherent assumption that their observable behavior accurately reflects their level of engagement; however, this may not be true (i.e., a student may display behaviors of a lower engagement level such as listening to other students but be silently making connections which is characteristic of a higher level of engagement). Furthermore, previous research shows that engagement is a multi-dimensional construct and that the individual dimensions are related; i.e., cognitive engagement is affected by behavioral and emotional engagement (Fredricks *et al.*, 2004; Naibert and Barbera, 2022). Therefore, it is possible that factors that influence behavioral or emotional engagement may indirectly impact cognitive engagement. Additionally, since only specific activities were selected for analysis based on the potential likelihood for a high level of group interaction, findings also cannot be generalized to all activities.

Data collection occurred during the COVID-19 pandemic when classes were held both in person and remotely. Although students did participate in group work, the interaction of groups may have been impacted by the remote environment. For example, it was more difficult for students to share what they were writing, i.e., they either held papers up to the camera or attempted to verbally describe what was on their paper. This restriction may have affected how students engaged in the activity. Finally, when making comparisons between different groups in the General Chemistry course, individual differences among students could contribute to the engagement modes observed.

Chapter 2: Review of the Literature

Introduction

Active learning (AL) has become a more prevalent teaching pedagogy in science, technology, engineering, and mathematics (STEM) classrooms in recent years. Studies of AL classrooms have repeatedly shown a positive relation between the implementation of AL and achievement outcomes as measured by exam scores, final course grades, and a reduction in course failure rates (Freeman *et al.*, 2014; Wilson and Varma-Nelson, 2016; Deslauriers *et al.*, 2019; Williams *et al.*, 2019). This improvement in achievement outcomes with AL was also found to differ based on demographics (Haak *et al.*, 2011). Additionally, in some instances, an increase in student failure rate with AL implementation was observed (Freeman *et al.*, 2014). In chemistry-specific classrooms, the magnitude of the effect of AL has been found to be dependent on the type of AL method being employed (Rahman and Lewis, 2020). Under the umbrella of AL, methods that included group work such as Process-Oriented Guided Inquiry Learning (POGIL) and collaborative learning had a positive effect on achievement outcomes (Rahman and Lewis, 2020). Because how students engage during group work could contribute to student success, understanding both the degree to which students engage and the factors that contribute to student engagement could help explain discrepancies seen in AL classes which incorporate group work.

Thinking about Student Learning

Early studies conducted in the 1980s and 1990s in chemistry courses demonstrated that students' achievement scores were higher on algorithmic problems than on conceptual problems (Nurrenbern and Pickering, 1987; Pickering, 1990; Sawrey, 1990; Nakhleh, 1993; Nakhleh and Mitchell, 1993; Salta and Tzougraki, 2011; Surif *et al.*, 2014). These results are consistent across General Chemistry and Organic Chemistry (Pickering, 1990), among low and high achieving students (Sawrey, 1990), and across multiple topics in General Chemistry (Nakhleh, 1993). Research suggests that algorithmic questions tend to promote lower-order thinking skills, such as memorization of procedural steps to solve a problem, whereas conceptual questions promote higher-order thinking skills, such as evaluating a problem and combining multiple pieces of information to develop a novel solution (Zoller *et al.*, 2002). In addition, these studies suggest that traditional instruction (i.e., lecture) does not effectively teach students these higher order skills (Zoller *et al.*, 2002). Therefore, there is a need to explore alternative instructional methods to fill this gap.

During the 1990s, there were also national calls for educational reform focused on a shift from teaching to learning (National Science Foundation, 1996; Boyer Commission, 1998) with a specific call for more student-centered instructional pedagogies (National Research Council, 1996). In a meta-analysis of group learning in STEM courses, Springer stated, "what students learn is greatly influenced by *how* they learn", and active learning experiences may be one way to more effectively influence how students learn (Springer *et al.*, 1999). Thus, there is a need to investigate more student-centered teaching pedagogies, such as AL.

Active Learning

An early definition states that AL "includes instructional activities involving students in doing things and thinking about what they are doing" (Bonwell and Eison, 1991). More recently, AL has been defined as "everything else that students could be doing while not being lectured, often doing collaborative/interactive activities in small groups or dyads" (Chi *et al.*, 2018). Because AL is so broadly defined, it encompasses many different techniques, from methods which include the whole class such as clicker questions or think-pair-share (TPS), to small group activities such as collaborative learning or POGIL.

Clickers are small, handheld devices which allow students to individually respond to a multiple-choice question posed by an instructor in a large classroom (Caldwell, 2017). This system allows all students to participate in answering the question as well as giving the instructor a quick assessment of the understanding of the material presented by the class as a whole. It can also reveal student misunderstandings of the material. However, because clicker questions are intended to give a brief glimpse of the state of the class, writing effective questions in a multiple-choice format which address higher order cognitive skills and conceptual knowledge may be challenging (MacArthur and Jones, 2008; Walvoord and Hoefnagels, 2011).

TPS is an active learning strategy consisting of three steps: 1) students individually think about a question posed by an instructor, 2) students work in pairs or small groups to discuss the question, and 3) the instructor calls on a subset of students to share their thoughts with the whole class (Lyman, 1981; Cooper *et al.*, 2021). Recent research into this method suggests that while the think and pair portions of this technique benefit students by allowing them to improve the complexity of their responses and practice communication with their peers in a low-stakes environment, the benefits to the share portion are less clear. Some concerns with the share portion of TPS include a lack of representation of the diversity of ideas exchanged during the pair discussion, lack of participation in the share due to anxiety in speaking in front of a large class, and whole class share discussion may be consistently dominated by a subset of students (Cooper *et al.*, 2021). AL techniques which incorporate small group work similar to what occurs in the pair portion of TPS may be beneficial without the concerns of the whole class share.

Collaborative learning is defined as "students working together toward a common goal using well-structured assignments that help guide a group of students toward a particular learning outcome" (Shibley and Zimmaro, 2002). In this environment, students are expected to mutually work together on problems, but their performance on the activity is evaluated individually, not as a group. Although multiple studies have demonstrated an improvement in course grades with collaborative learning, the magnitude of this improvement varies greatly from small to large effect size (Micari and Pazos, 2019; Rahman and Lewis, 2020). Additionally, there has also been a case of no measurable improvement with collaborative learning (Shibley and Zimmaro, 2002).

Process-Oriented Guided Inquiry leaning (POGIL) uses a structured format where the students in a group are assigned specific roles and engage in activities following a three-step learning cycle (Moog and Spencer, 2008; Rahman and Lewis, 2020). This cycle begins with an exploration step where students first cement their knowledge of basic concepts by answering questions based on a provided model. Second is the concept invention step where students investigate trends and patterns to further develop their understanding. The last step of the cycle is the application phase where the new concept is applied to problems in novel ways. Research on the effectiveness of POGIL implementation in chemistry classes indicates a positive relation on academic performance outcomes, both in small case studies (Ruder and Hunnicutt, 2008) and in large statistical analyses (Vincent-Ruz *et al.*, 2020). However, a meta-analysis conducted by Rahman and Lewis (Rahman and Lewis, 2020) of 99 chemistry classes suggests that although in general, the positive relation previously mentioned is confirmed, there may be some cases where implementation of POGIL results in no effect on performance outcomes.

Understanding what factors within an individual AL method contribute to improved achievement outcomes could help to minimize some of the discrepancies in outcomes observed across implementations of that method. In addition, understanding specific factors could allow for more effective design of future AL activities, specifically how such activities are both structured and how they are supported in the classroom. Research has shown that factors such as positive interdependence among students, face-to-face promotive interaction, and a high level of interpersonal and social skills are critical to a successful cooperative effort in a group activity (Johnson and Johnson, 1999), and it is possible that these traits are related to how engaged students are during the group learning activities.

Student Engagement

In general, studies of student engagement have shown a positive relation between engagement and achievement outcomes (Fredricks *et al.*, 2004; Kuh *et al.*, 2008; Lee, 2014; Wara, Aloka, *et al.*, 2018; Wara, Peter, *et al.*, 2018; Delfino, 2019; García-

Martínez *et al.*, 2021). Although the majority of these studies were conducted among secondary school students, there are a few studies showing a positive correlation between engagement and student grades among university students (Kuh *et al.*, 2005; García-Martínez *et al.*, 2021). A commonly used definition identifies engagement as a multi-dimensional construct with three dimensions: behavioral, emotional, and cognitive (Fredricks *et al.*, 2004). The behavioral dimension has been defined as what students are "doing" and includes behaviors such as participation and physical effort. The emotional dimension consists of what students are "feeling" and includes affective reactions such as boredom, interest, frustration, etc. The cognitive dimension conveys what students are "thinking" and relates to students' investment in comprehending the material and mastering knowledge. In addition to studies which relate engagement as a whole to achievement outcomes (Kuh *et al.*, 2008; Delfino, 2019; García-Martínez *et al.*, 2021), several studies have focused on how the specific dimensions of engagement relate to achievement (Lee, 2014; Wang *et al.*, 2015; Lei *et al.*, 2018; Wara, Aloka, *et al.*, 2018). However, there is limited work investigating *how* cognitive engagement affects achievement outcomes. Since working through group learning activities (e.g., collaborative learning or POGIL) involves learning and mastering the concepts being presented in the activity, investigation of how students' cognitive engagement varies during these types of activities may be important in understanding the role of engagement in the relation between group learning activities and improved student achievement outcomes.

Although Fredricks (Fredricks *et al.*, 2004) defined cognitive engagement as students' investment in mastery of knowledge, this definition is not consistently used throughout the literature. Additional definitions of cognitive engagement include “a willingness to engage in effortful tasks, purposiveness, strategy use, self-regulation” (Sinatra *et al.*, 2015) and “a type or degree of cognitive strategy use, use of self-regulatory processes and degree of effort exerted” (Greene, 2015). Appleton (Appleton *et al.*, 2008) related motivation to cognitive engagement by describing motivation as the “direction, quality, and intensity of one’s energies” and engagement as the “energy in action, [connecting the] person and activity. Pitterson (Pitterson *et al.*, 2016) related cognitive engagement to task complexity and mental exertion, and a review by Greene (Greene *et al.*, 2004; Greene, 2015) found cognitive engagement to be very complex, relating to motivation, mastery goals, and self-efficacy. Figure 2.1 presents a diagram displaying various components which could relate to cognitive engagement.

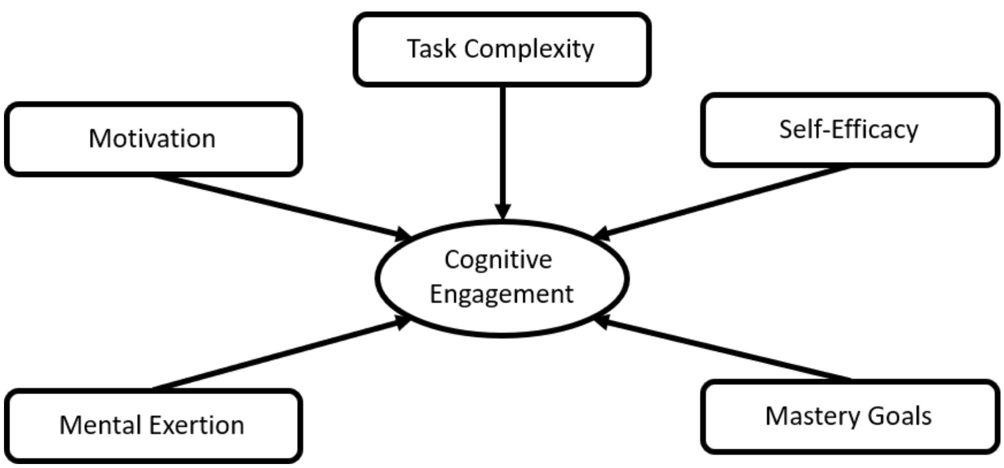

Figure 2.1: Possible components which can relate to cognitive engagement

Using these different definitions of cognitive engagement, multiple survey instruments have been developed. Appleton’s Student Engagement Instrument (SEI) used the concepts of self-regulation and strategy in his definition for cognitive engagement

(Appleton *et al.*, 2006). They used responses from eighth and ninth grade students to create self-report Likert scale items for the instrument. The Motivated Strategies for Learning Questionnaire (MSLQ) (Pintrich and De Groot, 1990) defined cognitive engagement as motivation and strategy use and was developed by administering self-report measures among seventh-grade students in English and science classes. The Learning and Study Strategies Inventory (LASSI) (Cano, 2006; Greene, 2015) identified cognitive engagement as using learning strategies and self-regulation and was designed to measure cognitive engagement through a self-report instrument among high school and college students. Barlow (Barlow *et al.*, 2020) developed the Student Course Cognitive Engagement Instrument (SCCEI) to measure modes of cognitive engagement defined as degree of peer interaction and notetaking in college engineering students. Naibert (Naibert and Barbera, 2022) developed the Activity Engagement Survey (AcES) to measure behavioral, emotional, cognitive and social engagement of students while working on active learning activities in general chemistry classes.

Survey instruments such as the SEI (Appleton *et al.*, 2006), MSLQ (Pintrich and De Groot, 1990), and the SCCEI (Barlow *et al.*, 2020) measure engagement at a large grain size; i.e., students retrospectively report on their behavior during class (Pintrich and De Groot, 1990; Appleton *et al.*, 2006) or when students are interacting with peers or taking notes (Barlow *et al.*, 2020). Therefore, they assume that cognitive engagement remains stable regardless of what the student is doing. Alternatively, Rotgans and Schmidt (Rotgans and Schmidt, 2011) developed an instrument to measure cognitive engagement during a specific task. The use of this instrument in a flipped learning classroom (Seery, 2015) showed a range of responses of students' perception of their own engagement while working on solving a problem in class. While the AcES instrument can investigate students' engagement during active learning activities while participating in group work, it combines behavioral and cognitive engagement into a single dimension (Naibert and Barbera, 2022). Furthermore, although survey responses provide quantitative methods to measure cognitive engagement by gathering information from a large number of students quickly and easily, they do not necessarily capture what is occurring in the individual groups (Miles *et al.*, 2014). In addition, quantitative responses to such self-report instruments can lack context as to how deeply students are engaging.

Whereas quantitative analysis is used to investigate trends across populations, qualitative research methods can aid in conceptual development and offer insights into context that are difficult to achieve using quantitative methods (Miles *et al.,* 2014; Hartig, 2021). Qualitative methods have been used in education research to investigate students' argumentation and reasoning patterns during group activities (Kulatunga *et al.*, 2013; Leupen *et al.*, 2020; Hunter *et al.*, 2021). Therefore, it is possible that the use of qualitative methods could similarly provide a deeper understanding of how students are cognitively engaging during group learning activities. This type of qualitative analysis would require the use of a rigorous theoretical framework which: 1) uses a consistent definition of cognitive engagement and 2) provides context and interpretation to the measurement of different engagement modes.

Interactive-Constructive-Active-Passive (ICAP) Framework

Measuring cognitive engagement qualitatively is difficult without something concrete to observe. To address this issue, the Interactive-Constructive-Active-Passive

(ICAP) framework was developed to define and categorize different modes of cognitive engagement by observing students' overt behaviors (Chi, 2009; Chi and Wylie, 2014; Chi *et al.*, 2018). In this framework, cognitive engagement is defined as "the way a student engages with the learning materials in the context of an instructional or learning task" (Chi and Wylie, 2014), which aligns with Fredricks' (Fredricks *et al.*, 2004) definition of cognitive engagement as the student's investment in the comprehension of learning material and mastery of knowledge. Therefore, ICAP can be used to investigate the mastery goals component of cognitive engagement (Figure 2.1). This framework identifies four different engagement modes, with each mode being defined by specific observable behaviors. "Passive" engagement is defined as students simply receiving information without performing any overt action, for example, listening to a lecture. "Active" engagement involves some type of physical manipulation while learning, such as highlighting or underlining a text. "Constructive" engagement encompasses the physical manipulations which define the active mode; however, the students will generate output beyond the information provided in the learning material. This would include behaviors such as summarizing a text or taking notes in one's own words. "Interactive" engagement generates new content ideas like constructive engagement, but the generation of new information occurs through dialoguing between students or between students and instructors. Previous research suggests that positive interdependence (i.e., the perception that students are linked such that one cannot succeed unless the other does), face-to-face promotive interaction (i.e., the idea that students promote each other's success by encouraging each other's efforts to succeed), and social skills (e.g., such as teamwork and conflict resolution) are critical to the success of group activities (Johnson and Johnson, 1999). These variables can be used to support the identification of the interactive engagement mode during group activities. ICAP hypothesizes that students' mode of cognitive engagement increases as one moves from passive to active to constructive to interactive. The ICAP modes are depicted in Figure 2.2.

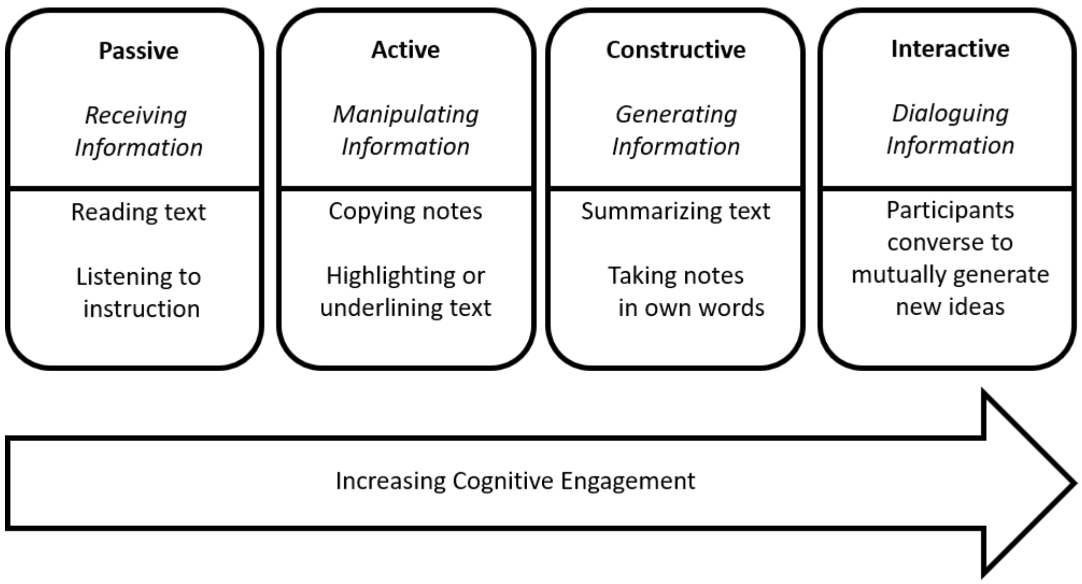

Figure 2.2: Modes of cognitive engagement according to the ICAP framework (Chi et al., 2018)

Application of ICAP to different classrooms suggests that the nature of group work promotes an improvement in learning outcomes with interactive modes of engagement. Analysis of a nonmajors biology class demonstrated that students working in groups (Interactive mode) performed better than students working alone (Constructive mode) (Linton *et al.*, 2014; Hodges, 2018). In a genetics course, groups of students who all answered a clicker question incorrectly and then discussed their answers (Interactive mode) were then more likely to answer a follow-up isomorphic question correctly (Smith *et al.*, 2009; Hodges, 2018). In an introductory biology class, the application of a jigsaw structure to an activity where each student learned a sub-topic and subsequently taught it to their peers (Interactive mode) showed a significant difference in learning gains over students who engaged in the activity without being required to interact with their peers (Constructive mode) (Wiggins *et al.*, 2017). These results suggest that ICAP can be used to understand how cognitive engagement during group learning activities relates to achievement outcomes. However, while ICAP defines interactive engagement as dialoguing between participants, all the studies discussed thus far have made assumptions about the students' interactive engagement without actually analyzing the context of any overt behavior such as the group conversations that occurred during each activity.

According to the ICAP framework, students who display Interactive engagement are engaging at the highest mode. One can identify Interactive engagement by analyzing the conversations that occur during group activities. Analyses done in an evolutionary biology course (Wiggins *et al.*, 2017) and a materials science course (Menekse and Chi, 2019) used observational protocols which involved measuring time spent interacting with other students to define Interactive engagement. The Interactive engagement of students in the biology class (Wiggins *et al.*, 2017) was measured as the number of times students talked or listened to another student or shared a worksheet with another student. In the materials science class (Menekse and Chi, 2019), Interactive engagement was defined by measuring the amount of time each student contributed to the conversation. Both of these studies attempted to identify Interactive engagement by analyzing group conversations; however, they did not look at the content of the conversation. It is possible that although students are contributing to the conversation, no co-generation of new information is occurring, which is a key component of Interactive engagement according to ICAP. Therefore, it seems inadequate to assume students engaged at the Interactive mode based simply on quantitative values such as duration length or frequency of student contribution. All the studies discussed thus far have made conclusions about the students' Interactive engagement without analyzing the content of any overt behavior.

In addition, although the ICAP framework identifies cognitive engagement through students' overt behaviors, many studies to date have used it to identify a *predicted* engagement level based on the activity being presented (Menekse *et al.*, 2013; Chi and Wylie, 2014; Wiggins *et al.*, 2017; Henderson, 2019; Barlow *et al.*, 2020). A study of high school physics classes (Henderson, 2019) using Peer Instruction implemented different instructional methods prior to students answering clicker questions. These methods were coded according to ICAP, where listening to a lecture was identified as Passive engagement and individually writing an answer to a problem was considered Constructive. However, students' overt behaviors were not observed. Furthermore, analysis of cognitive engagement using ICAP in an evolutionary biology (Wiggins *et al.*, 2017) and materials science (Menekse *et al.*, 2013) course related predicted engagement modes to achievement outcomes. In the biology course (Wiggins *et al.*, 2017), cognitive engagement in Constructive and Interactive activities was compared. In the Constructive activity, students were asked to generate new information by using compare and contrast mechanisms and making predictions. In the Interactive activity, students participated in a jigsaw activity where each student learned a sub-topic and subsequently taught it to other group members. Although students worked in small groups for both activities, interaction with other group members was not required for the Constructive activity. Results suggested that the Interactive activities resulted in a significant difference in learning gains over the Constructive activities, supporting the

ICAP hypothesis. Although both activities were conducted in small groups, no investigation into the content of conversation was done to determine if students truly engaged at the Constructive or Interactive mode. In the materials science class (Menekse *et al.*, 2013; Chi and Wylie, 2014), activities dealing with crystal structures and unit cells were classified according to ICAP. Active activities asked students to copy information from a unit cell diagram onto a blank piece of paper and Constructive activities asked students to construct unit cells given specific indices. Interactive activities asked students to make calculations regarding the number of atoms in a unit cell to investigate the cell's properties. In order to classify these activities as Interactive, students were asked to discuss the decisions they made with one another. Although these classifications align with ICAP, they were based on a prediction of how students would engage with the activity; however, students' overt behaviors were not observed. Even with assigning ICAP modes to the activity based on predicted student behavior, the results still confirmed an increase in student achievement with predicted engagement, supporting the ICAP hypothesis. Increasing engagement to the next consecutive mode showed a significant increase in learning gains across all modes with a medium effect size (Menekse *et al.*, 2013). Although the results of these studies suggest that increasing cognitive engagement does improve the effectiveness of group learning activities, their application of the ICAP framework *assumed* specific engagement modes instead of identifying overt student behaviors.

Further review of these studies revealed that they also assigned a single engagement mode to an entire activity, which may be inaccurate as students could engage with different parts of an activity using different engagement modes. There has been limited research using ICAP to examine cognitive engagement at a finer grain size. In a study conducted in a Physical Chemistry class, a modified form of ICAP was used to identify engagement (Liyanage *et al.*, 2021). Verbal interactions were analyzed, and a single engagement mode was identified over the course of a conversation which may have included multiple questions; however, it is possible that students' engagement changed across the different questions. Additionally, this study only focused on *one* student's statements when categorizing engagement level; thus, Interactive engagement may have been coded incorrectly as it is defined as the co-dialoguing between students.

By applying ICAP in the ways summarized above, researchers assume, perhaps erroneously, that students will 1) engage at a single mode over the course of an activity, and 2) engage at the mode assigned to the activity without evidence of any overt behavior. In order to analyze an overt behavior such as conversations during group activities, specific methods to study verbal interactions are needed. Qualitative techniques such as thematic analysis and conversation analysis could provide insight into the content of conversation during group activities (Hsieh and Shannon, 2005; Clayman and Gill, 2012; Greene, 2015; Braun and Clarke, 2020). These methods in combination with the ICAP framework can be used to investigate student engagement during group activities.

Qualitative Methods

Most qualitative data analysis involves the examination of text-based data sources, which include transcripts from interviews or recorded observations, written responses to survey questions or journal entries (Suter, 2012). Analysis of these sources has the goal of gaining insight into patterns or themes that may emerge from the text under investigation. In education research, interviews and recorded observations are the primary sources of qualitative data. Although interviews can provide complete in-depth data in an interactive environment where the interviewer can probe for clarity, this method also has some well-defined limitations (Alshenqeeti, 2014). These limitations may include faulty memory and subconscious bias on the part of the interviewee. Therefore, if interviews are used to study group interactions during an active learning activity, it is possible that students may not remember specific actions or statements during the course of the activity or that students may reveal only specific perceptions of occurrences during the activity, thereby giving a subjective viewpoint.

In contrast, recorded observations provide a permanent account of a transient situation which includes both verbal and non-verbal behaviors (Latvala *et al.*, 2000; Simpson and Tuson, 2003; Caldwell and Atwal, 2005). Information from recorded observations is more detailed and direct than information that is obtained from interviews. Use of recordings also creates a more credible result by allowing multiple researchers to examine the same recording, known as investigator triangulation (Lincoln and Guba, 1985), or allowing the application of multiple analytical techniques to the same data source, known as analysis triangulation (Hussein, 2009). Additional advantages of the use of recorded observations include minimizing self-report fatigue that may occur with interviews, reducing participant bias, i.e., students may not tell the interviewer all the information relevant to a specific phenomenon, and the ability to repeatedly watch the recordings for a complete thorough analysis (Latvala *et al.*, 2000; Caldwell and Atwal, 2005).

Recordings of small group conversations during active learning activities can be investigated to determine how cognitive engagement of students as individuals and as a group change during the course of the activity. Discourse analysis has been used extensively in chemistry education research to study small group work in different AL environments (Krystyniak and Hekkinen, 2007; Young and Talanquer, 2013; Becker *et al.*, 2015; Moon *et al.*, 2016; Repice *et al.*, 2016). Discourse analysis is generally defined as investigating "texts and talk in social practice" (Wood and Kroger, 2000); in an educational context, Cole (Cole *et al.*, 2014) defines it as a family of approaches used in the analysis of verbal or written language. Analytical techniques include thematic analysis (TA) and conversation analysis (CA). Thematic analysis is a broad analytical method which involves interpretation of the content of text sources to identify patterns and grouping of identified patterns around a central idea or theme (Braun *et al.*, 2019; Pearse, 2019; Braun and Clarke, 2020). The coding of segments of text with similar patterns into specific categories is sometimes called content analysis (Hsieh and Shannon, 2005). In psychological literature, content analysis has also been called the constant comparison technique. Leech et al. (Leech and Onwuegbuzie, 2008) defined constant comparison as a systematic approach of coding and categorizing textual data to understand multiple meanings. For the purposes of this dissertation, the analytical approach of coding data into categories and subsequently assigning themes to the categories will be referred to as thematic analysis. In contrast, conversation analysis does not look at *what* is being said but instead examines talk for *how* people produce social interaction (Leech and Onwuegbuzie, 2008). Conversation analysis identifies specific features in talk such as gaps and overlap (participants speaking at the same time) to understand the participants' actions (Sert and Seedhouse, 2011; Strauss and Feiz, 2014).

Application of Thematic and Conversation Analysis in Education Research

Several studies in chemistry education applied thematic analysis to the investigation of student problem solving and reasoning. A study of a Peer-Led Team Learning (PLTL) chemistry classroom used thematic analysis to investigate types of student talk which develop problem-solving skills (Repice *et al.*, 2016). The study produced a variety of codes from the conversation student groups participated in while solving specific chemistry problems. Analysis of the codes suggested that student talk could be divided into two categories: regulative talk, consisting of conversation which aided the groups in working collaboratively, and instructive talk, consisting of chemistry-content related conversation. Investigation of student discourse using thematic analysis during small group POGIL activities in a Physical Chemistry class found that students consistently use particulate-level reasoning to explain chemical and physical properties (Becker *et al.*, 2013). Thematic analysis was also used to analyze student-instructor verbal interactions in order to understand the nature of levels of confusion in an open-inquiry General Chemistry lab (Krystyniak and Hekkinen, 2007). Student conversations during group activities using thematic analysis across multiple studies have also shown that higher-order questions promote argumentation, meaning-making talk, and increased conceptual learning, whereas lower-order questions have more procedural and off-topic talk (Osborne, 2010; Young and Talanquer, 2013; Repice *et al.*, 2016; Leupen *et al.*, 2020). In addition, thematic analysis of small group conversations in an introductory chemistry course suggested that more exploratory activities promoted higher levels of meaningful engagement with course content than commonly used data analysis activities

(Young and Talanquer, 2013). These results show that qualitative methods such as thematic analysis can be used to identify types of talk that students use to solve problems. It is possible that these methods could also be used to investigate what role cognitive engagement may play in the relation between activity design and higher and lower-order thinking.

Outside of chemistry education, research in an undergraduate biology lab used thematic analysis to explore the different ways students engage in group conversation and what effect group dynamics have on these conversations (Paine and Knight, 2020). A study in an undergraduate physiology class used thematic analysis and the ICAP framework, to investigate the relation between the complexity of questions being asked and the level of student engagement (Leupen *et al.*, 2020). Results indicated that higher-level questions promoted an increase in interactive conversations that focused on conceptual explanations.

While thematic analysis has been used in chemistry education research to examine what students are saying to understand how they solve problems, there is a distinct lack of the use of conversation analysis (CA) to investigate how students interact with one another. However, CA has been used in other education research. For example, one study investigated how language teachers' perception of the knowledge they bring to a classroom as documented through journal entries differed from how that knowledge actually manifested during classroom communicative practices (Fagan, 2012). Comparison of journal entries with CA of the classroom discourse indicated instances of both complementary and contradictory findings between the two sources. A different study explored the strategies parents who self-identified as engineers employed while reading an engineering storybook to their children (Brinkman and Louise, 2015). Use of CA found that the interaction between parent and child was shaped by the parents' background, attitudes, and beliefs.

The majority of work looking at group conversations in STEM courses investigated the content of these conversations to make conclusions regarding student reasoning; a similar analysis could be used to examine cognitive engagement in group activities.

Engagement, Discourse, and Cognitive Load

In the ICAP framework, the highest mode of engagement, Interactive, involves discourse between the students or instructors (Chi *et al.*, 2018). Small group work is a learning environment that lends itself to students engaging in the Interactive mode because students work together and converse to solve problems. Exploration of the conversations that occur can provide insight into where and how students struggle on activity worksheets.

Students' struggle in mastering new material can be analyzed through the lens of cognitive load theory (CLT). This theory claims that the capacity of an individual's working memory is limited, and when the capacity or cognitive load needed to master new information exceeds the capacity available in the working memory, learning is hampered (Paas *et al.*, 2003; de Jong, 2010). Therefore, in order to optimize learning, CLT attempts to design instructional systems to reduce cognitive load. Three types of cognitive load exist: 1) intrinsic load is the difficulty of the subject material and includes the number of elements that interact to comprehend the material, 2) extraneous load, which includes the load caused by aspects of the instructional design which do not contribute to learning, and 3) germane load, which consists of the learning processes that students use, such as interpretation, classification, and organization (de Jong, 2010). By analyzing group conversations for elements that contribute to cognitive overload, this information can be used to design and modify items in activity worksheets to reduce the overload and optimize student learning.

Trustworthiness

In qualitative research, trustworthiness is used to evaluate if the results of the study can be trusted; this is established through quality criteria such as credibility, transferability, dependability, and confirmability (Lincoln and Guba, 1985; Korstjens and Moser, 2018). Credibility provides confidence that the research findings represent a correct interpretation of the participants' original views. This is established through prolonged engagement with the participants through observations or interviews, and through triangulation. Data triangulation involves using multiple data sources (i.e., recorded observations and interviews) and investigator triangulation uses multiple researchers to analyze the data. Transferability is how applicable the research study may be to other settings. It is established through a "thick description", i.e., clear details of the participants and research process, which would allow other researchers to determine if the findings would be applicable to their own setting. Dependability looks at consistency or repeatability of the results. This is accomplished through an audit trail, i.e., a complete record of all decisions made throughout the research process. Confirmability is defined as the objectivity or neutrality of the data. This can be evaluated by determining qualitative reliability. Reliability is generally defined as the consistency of a specific measurement. When looking at qualitative data and a set of codes, it is important to reduce the subjectivity of code assignments by employing more than one coder to evaluate the data. Inter-coder reliability (ICR) is a quantitative measure of the level of agreement between coders and can help improve the trustworthiness of the analysis (O'Connor and Joffe, 2020). The most commonly reported measure of ICR is the percentage of data units where the coders agree; however, there is concern that these values are overestimated due to some percentage of agreement between coders occurring by chance (Cohen, 1960; Hallgren, 2012). To correct for the possibility of chance agreement, rigorous statistical measures are available such as Cohen's kappa (κ). Kappa values of greater than 0.8 are generally considered to show good reliability (Landis and Koch, 1977).

Chapter 3: Methods

As active learning, and specifically active learning which incorporates group work, becomes more prevalent as an instructional pedagogy, it is important to understand the specific elements which make it effective in the classroom. While there are many possible elements that could contribute to the success of AL, this project focused on investigating the different levels students cognitively engage at and what factors may influence the differences observed in students' cognitive engagement. These goals were addressed by the following research questions:

RQ 1. a) How do student groups' expected and observed cognitive engagement align while participating in small-group active learning activities in chemistry courses?

b) What themes may contribute to any observed misalignment?

RQ 2. a) How does individual students' cognitive engagement vary while participating in small-group active learning activities in chemistry courses?

b) What factors may affect individual students' cognitive engagement?

RQ 3. What relations are observed between the type of question asked in the activities and students' level of cognitive engagement?

RQ 4. a) How can analysis of group conversations inform improvements to learning activities to enhance student understanding?

b) What improvements can be made to learning activities to enhance student understanding?

Chapter 4 will look at the engagement of the group as a whole and investigate the alignment of expected and observed engagement (RQ1). In Chapter 5, a finer grain size will be explored, where each individual student's engagement is analyzed and trends in engagement based on various factors are investigated (RQs 2 and 3). Chapter 6 will focus on the activity itself and how its structure influences student understanding (RQ4).

Human Subjects Research

All parts of this project that involved human subjects received Institutional Review Board (IRB) approval (HRPP# 207004-18 and 217370-18).

Activities

In order to gather a reasonable number and variety of group conversations for analysis, up to three activities were selected during each term of data collection in General Chemistry and Physical Chemistry classes. Activity selection was based on the likelihood that the activity would promote group conversation between multiple students based on the type and complexity of questions being asked. The Molecular Polarity activity used in Fall 2021 was a modified version of the Electronegativity and Polarity activity used in Fall 2020. Group conversations during Fall 2020 were analyzed, and select questions were removed so that the activity could be completed in a single class session. The Hydrogen Atom and Harmonic Oscillator activities that were used in Spring 2022 are also modified versions of the same activities that were used in Spring 2021. In the new versions, based on analysis of group conversations in Spring 2021, new models were added to the activities, questions were rigorously scaffolded, and conceptual questions were added to promote an improvement in student understanding. Table 3.1

shows the activities that recordings were collected from during the 2020-2021, 2021-2022, and 2022-2023 academic years.

Table 3.1: Activities used for data collection

Honors General Chemistry		**General Chemistry**		**Physical Chemistry**	
Fall 2020	***Winter 2021***	***Fall 2021***	***Fall 2022***	***Spring 2021***	***Spring 2022***
Mole and Molar Mass	Thermal Energy and Calorimetry	Solutions and Dilutions	Solutions and Dilutions	Hydrogen Atom	Hydrogen Atom*
Solutions and Dilutions		Limiting Reactants	Periodic Trends and Electron Configuration	Harmonic Oscillator	Harmonic Oscillator*
Electronegativity and Polarity		Molecular Polarity**	Molecular Polarity**		

*These activities are modified versions of the same activity run the prior year

**The Molecular Polarity activity is a modified version of the Electronegativity and Polarity activity

All activities for General Chemistry and Physical Chemistry were created in house at PSU. In the Honors General Chemistry class, the instructor gave a short lecture introducing concepts in the activity prior to groups starting to work on the activity, and in the General Chemistry class, there was minimal lecture prior to the start of the activity. Activities were implemented during a single day in both classes. The activities consisted of models, key questions (KQ), exercises (E), and problems (P). The models contained conceptual information needed to answer the questions in the activity. Key questions were generally simple questions which could be answered with information explicitly present in the model, exercises asked students to perform a calculation or make an inference based on model content, and problems were multi-step questions or asked students to use the model in an original way.

In the Physical Chemistry class, there was a short lecture each day introducing concepts prior to the start of the activity. The Hydrogen Atom activity was implemented over multiple days, and the Harmonic Oscillator activity was done in a single day. The activities used in Spring 2021 did not contain models; instead, the questions were based on material presented in lecture. The re-worked versions of the Hydrogen Atom and Harmonic Oscillator activities which were implemented in Spring 2022 contain simple models provide key equations and relations necessary to answering the questions. The re-worked Harmonic Oscillator activity labeled the questions as key questions, exercises, and problems in a similar manner to the General Chemistry activities; however, in the Hydrogen Atom activity, due to the large amount of content and complexity of the different types of question being asked, the key question, exercise, and problem labels were not used.

Group Recordings

Participants

The initial sample pools were created using convenience sampling. This is a sampling technique which uses a period of open recruitment among subjects of the population that are easily accessible to the researcher (Luborsky and Rubinstein, 1995; Etikan *et al.*, 2016). For this project, the population was students in either General Chemistry, Honors General Chemistry, or Physical Chemistry classes. Since data was collected during the COVID-19 pandemic, recordings occurred in both in-person and remote classes that were held through the Zoom platform. For in person classes, up to two groups could be recorded due to the numbers of cameras available. For remote classes, up to three groups could be recorded due to the numbers of researchers available to record breakout rooms. Observed groups were capped at a maximum of five students to increase the likelihood of interaction and conversation occurring among all group members. When the number of students in the convenience sample was larger than the number of students possible based on the maximum number of groups, quota sampling was used to reduce the sample size. Quota sampling selects participants to ensure representation of all groups (Luborsky and Rubinstein, 1995; Sharma, 2017). In this project, it was used to ensure inclusion of underrepresented groups based on gender identity and race/ethnicity. Once a sample pool was established, students were randomly assigned to groups using Google's random number generator.

For the Fall 2020 Honors General Chemistry and Spring 2021 Physical Chemistry classes, recruitment occurred at the beginning of the term, and the convenience sample pool did not require any additional reduction. For the Fall 2020 Honors General Chemistry class, students who consented were randomly assigned to a specific group by the instructor. The students then participated in the same groups for all three observed activities. For the Spring 2021 Physical Chemistry class, the student groups were consistent throughout the term; however, on observation days, these groups were changed so that consenting students were grouped together. The groups on observation days were the same for all observed activities. During the 2021-2022 and 2022-2023 academic years, for the General Chemistry class, students consented prior to each activity, and group makeup was not consistent throughout the term. Therefore, group assignment occurred using the Google random number generator for each observed activity. For the Spring 2022 Physical Chemistry class, students consented at the beginning of the term to be observed, and the consenting groups were kept consistent for the entire term. The course, term and modality (remote vs. in person), activity and number of students in each observed group are shown in Table 3.2.

Table 3.2: Course type, term, modality, activity, and number of students per group recorded for data collection

Course	Term and Modality	Activity*	# participants per group
General Chemistry	Fall 2020 Honors (remote)	MM	3
			3
		SD	3
			3
		EP	3
			3
	Winter 2021 Honors (remote)	TEC	3
	Fall 202 Dr. Green (remote)	LR	4
			4
			5
		MP	4
			4
			3
	Fall 2021Dr. Black (in person)	SD	4
			4
		LR	4
			5
		MP	3
			5
	Fall 2022 (in person) Dr. Red	SD	2
			3
		PT	3
			2
		MP	2
	Fall 2022 (in person) Dr. Black	SD	4
			4
		PT	3

			5
		MP	2
			2
Physical Chemistry	Spring 2021 (remote)	HA	2
			3
		HO	2
			3
	Spring 2022 (in person)	HA	3
			3
		HO	3
			3

*MM = Mole and Molar Mass, SD = Solutions and Dilutions, EP = Electronegativity and Polarity, TEC = Thermal Energy and Calorimetry, LR = Limiting Reactants, MP = Molecular Polarity, PT = Periodic Trends, HA = Hydrogen Atom, HO = Harmonic Oscillator

Data Collection

Due to the COVID-19 pandemic, recordings of group work occurred during remote and in-person classes. In the remote environment, consenting students were placed together in a breakout room, and they kept their cameras and microphones on. A researcher was also present in the breakout room (with their camera and microphone off) to record the group. For the in-person environment, two video cameras were placed on opposite sides of the group for recording in order to capture all the voices conducting conversation equally.

During the 2020-2021 academic year, data was collected during the Honors General Chemistry and Physical Chemistry class which were all held remotely. During the Fall 2021 term, data was collected in two sections of General Chemistry, where one section was conducted in a synchronous format remotely and the other section was held in person. Due to technical difficulties recording with Zoom, no data was collected during the Solutions and Dilutions activity in this class. In addition, observed groups in this class tended to work silently on their worksheets with very little interaction between students. For this reason, data from this class was not used in any analysis. During the first two activities of the in-person General Chemistry class in the Fall 2021 term, it was difficult to hear and understand the conversation between students due to the high level of background noise in the classroom and the muffling effect of students wearing masks. Therefore, from the third activity of Fall 2021 and onward, two audio recorders were placed on a table in the center of the group facing opposing directions to obtain clearer audio recordings. During the Fall 2022 term, data was collected in two sections of General Chemistry, one taught by Dr. Red and one taught by Dr. Black. Both instructors implemented the activity in a similar manner with minimal in-class instruction and the bulk of the class time was spent working on the activity worksheets in small groups.

Recordings were transcribed first using an automated transcription service (TEMI). The transcripts were then cleaned by a chemistry or linguistics researcher. Cleaning included identifying a change in speaker and editing incorrectly transcribed content.

For the General Chemistry class during the Fall 2021 and Fall 2022 terms, activity worksheets were also collected as an additional data source. During the Fall 2021 term, students were asked to email a copy of their worksheet to the researcher after the observed class period was over. However, students were inconsistent about emailing their worksheets, and in some instances, students completed the worksheet on their own prior to emailing their copy. By doing this, it was difficult to determine which answers occurred during group work. For this reason, during the Fall 2022 term data collection, the researcher collected the worksheets at the end of the group work and emailed students a copy of their worksheet by the end of the day.

Interviews

Interviews were conducted among students who participated in the recorded groups to supplement knowledge obtained from the group recordings by gaining insight into students' perceptions of how the activity influenced students' understanding of the material presented.

Participants

For the Spring 2021 Physical Chemistry class, students who participated in recorded groups during the Hydrogen Atom activity were emailed a request for an interview immediately after the activity was completed. Interviews were then conducted one week after the activity. All students who consented participated in an interview. For the Fall 2021 General Chemistry class, students were interviewed after the term ended. At the beginning of the Winter 2022 term, emails were sent to students who participated in at least two of the three activities, and the interview covered all activities the student participated in. Since these interviews occurred 3-6 weeks after the activity occurred, students seemed to have difficulty recalling specific details about work on the activity and group interactions. Therefore, in the Spring 2022 term and the Fall 2022 term, interviews were conducted on up to two activities per term and within one week following the activity.

Data Collection

Interviews were conducted using a semi-structured format. This type of interview begins with a pre-determined set of questions but allows for flexibility of follow-up questions for an in-depth exploration or clarification as needed (Herrington and Daubenmire, 2014). The full set of interview questions can be found in Appendix A. Interviews were conducted and recorded remotely using the Zoom platform. Recordings were then transcribed and cleaned using the same method as with the group recordings.

Data Analysis Techniques

Recordings were analyzed using deductive and inductive coding. A code is a word or phrase which captures the interpreted meaning of a portion of text (Saldaña, 2013). Coding then refers to the process of assigning codes throughout the text of interest. Deductive coding applies a pre-determined set of codes to the data whereas in inductive coding, the codes emerge from the data itself (Bingham and Witkowsky, 2022). This project used thematic analysis which falls under the general umbrella of inductive and deductive coding. This technique was used to investigate what was being said during group conversations or interviews and how the conversations showed evidence of cognitive engagement. In addition, conversation analysis was used to examine specific features of the talk in group conversations to understand how the manner students interacted with one another may have affected their engagement.

Thematic Analysis

Thematic analysis (TA) identifies patterns among codes and groups similar codes together around a central organizing concept or "theme" (Braun *et al.*, 2019; Pearse, 2019). A number of different methods, both inductive and deductive, exist under thematic analysis. The "coding reliability" TA method, also known as directed content analysis (Hsieh and Shannon, 2005), uses a deductive approach where a codebook is developed based on an existing theoretical framework. The codebook is then applied to the text and revised as needed. Multiple coders are used in this method to minimize the threat of researcher subjectivity in the interpretation of the data. Under coding reliability TA, themes are simply summaries of the things most frequently said with little interpretation involved in theme development (Pearse, 2019; Braun and Clarke, 2020). “Codebook TA”, or conventional content analysis (Hsieh and Shannon, 2005), is a second method that extends coding reliability TA by starting with the deductive approach to group similar codes together but then uses inductive coding to develop new themes by examining the codes for similar patterns. With codebook TA, the themes are determined by both the researcher’s objective and their interpretation of the patterns of shared meaning (Thomas, 2006; Braun *et al.*, 2019).

Conversation Analysis

Conversation analysis (CA) focuses on understanding participants’ actions by looking at the talk that occurs (Sert and Seedhouse, 2011). CA uses a detailed set of conventions for transcribing features of spoken language such as turn-taking, pauses and gaps in conversation, repair (participants correct misunderstandings to get conversation back on track), and overlap (participants speaking at the same time) (Strauss and Feiz, 2014; Hartig, 2021). This type of analysis can be used to understanding students’ engagement by exploring the strategies participants use to interact with one another (Halpin *et al.*, 2021). Additionally, what students mean can be analyzed by investigating their actions (Ingram, 2021). Such actions may include non-verbal behaviors such as eye gaze (where they are looking during the conversation), timing (at what point during the conversation students write their answers), and the content of their written responses on their worksheets.

Coding using the ICAP Framework

The Interactive-Constructive-Active-Passive (ICAP) framework was used as a basis for coding both the questions in the activities and the responses. The grain size was at the item level, where the unit of analysis was an individual item or part of an item in multi-part items. Coding of responses was done for both the group as a whole and for each individual student within the group.

Question Coding

For all observed activities, each item was coded based on the intended engagement of student groups. The code was identified by examining the item and determining how the answer would be generated by the group. The Passive mode of engagement from ICAP was not used as a code. Since the items were designed for use in a *group* activity, it was expected that students would work together and therefore, the group's lowest level of engagement should be Active. Items were coded as Active (A) if the answer was provided within the activity (i.e., within a model). According to ICAP, both Constructive and Interactive engagement involve the generation of new knowledge; however, in Interactive engagement, the knowledge is co-generated by more than one student where each students' contribution builds on the statement made by the previous student. This difference cannot be distinguished by looking at the item alone; therefore, Constructive and Interactive engagement were collapsed into a single code for question coding, Constructive/Interactive (C/I). Items were coded as Constructive/Interactive (C/I) if the answer to the item required the generation of new knowledge beyond the information provided in the activity models.

Response Coding

For both group and individual level response coding, the highest mode of engagement shown by the group or individual in their response to a specific item was identified as their engagement mode for that response.

Group Level

For all observed activities, the Passive mode of engagement was not used as a code since it was expected that students converse as a group (at least some fraction of them) to determine an answer, and because the act of conversation involves manipulation of information, students would engage at the Active level at a minimum. The engagement of the group as a whole was determined by looking at the entire conversation to answer the item. Regardless of the differing engagement levels of each student, the engagement of the group was determined by the highest engagement level that occurred during the conversation. If students explicitly referred to information in the model to answer the item, the group response was coded as Active (A). If only a single student generated new information to answer the question, the response was coded as Constructive (C). If conversation among the group occurred and involved only agreement such as head nods or saying “Yes” or “uh huh”, this was still coded as Constructive since the conversation did not co-generate any new information. The group response was coded as Interactive (I) if the conversation between students generated new information where more than one student contributed to the new information and the contributions from each student built upon one another.

Individual Level

For each group response to an item, each individual student's engagement level was determined. Within each group response, the statements made by an individual student, their physical actions, and their written responses on their activity worksheets were examined to evaluate that individual's engagement level. Students who did not participate in conversation, were not looking at other group members (i.e., looking at their phone), or did not appear to be working on the activity were coded as Unengaged (U). If students did not converse with other group members but appeared to be listening the group conversation (i.e., they are looking at the group and may nod in agreement) but did not seem to be working on the activity in any visible way, they were coded as engaging at the Passive (P) level. An individual was coded as Active if their statements referred to the model or they repeated statements made by another student without the generation of new information. If a student's statements or gestures of agreement with another student's Active or Constructive statement, the student's engagement level was also identified as Active. Additionally, if a student listened to the group conversation and subsequently wrote their answer on their worksheet or the student's written answer reflects the content of the conversation, this was identified as Active engagement. An individual's engagement level was coded as Constructive if that student generated new information to provide an answer without contributions from other students in the group. This may occur if one student "teaches" and the other students are "catching up". If conversation is about how to solve a problem, and each student subsequently writes on their worksheet or the written responses show that each student independently generated their own answer, each student in the group would be engaging at the Constructive mode. The engagement level of individual students was coded as Interactive if the student's statements generated new knowledge during conversation with other students, learning assistants, or the instructor. During conversation between students, the knowledge of more than one student increases. During conversation with learning assistants or instructors, the conversation co-generates information for the entire group. The codebooks for question, group response, and individual level coding are shown in Table 3.3.

Table 3.3: Codebook for question, group response, and individual level coding

Level	Code	Description
Question	Active (A)	• Information to answer the question can be found in provided models.
	Constructive/Interactive (C/I)	• New information needs to be generated to answer the question prompt.
Group Response	Active (A)	• Conversation reflects that an answer was taken from information provided in the models.
	Constructive (C)	• One person provides the answer, generating new information. • Can include forms of agreement from other group members (e.g., head nods, "yeah", "uh-huh").
	Interactive (I)	• Participants generate information to answer the question based on one another's responses. • Other participants' contributions of off-topic talk or forms of agreement are not included in this code.

Individual	Unengaged (U)	• Student does not appear to be working on the activity.
		    ○ Makes statements unrelated to activity.
		    ○ On their phone.
		    ○ Other behaviors unrelated to working on the activity.

	Passive (P)	• Student's gaze is directed towards other group members or activity worksheet. • Student may nod in agreement with the conversation regarding the activity but does not orient to the content of the activity in any visible way (e.g., they do not write down any information, do not point to specific parts of the activity).
	Active (A)	• Repeating content from the activity or repeating a statement made by another student in reference to a

		simple idea (i.e., identifying and writing down something specific from an equation or model). • Statements or gestures of agreement with an answer provided by another student (e.g., nodding while writing down an answer, giving a "thumbs up"). • Other evidence of orienting to the content of the activity but without generating new information (e.g., asking what number they are on). • Students listen to statements/conversation occurring among others students (i.e., orienting to the question) and then write their answer on their worksheet, and/or their written response on the worksheet reflects the content of the conversation.

	Constructive (C)	• Student provides an answer to question, generating new information independent of other members in the group.
		  ○ This may take the form of a statement or a request for confirmation. Other students may agree with the original student's statement and provide evidence of their own generation of information which does not add any new information to the group.
		  ○ If a single student's knowledge increases through dialogue, but the group's does not, this would be Constructive for that student. (If one student has the answer and "teaches" and others are learning or "catching up", the original student is Constructive).
		  ○ If the conversation is about how to solve the problem, and the students write after the discussion, we can assume each student is independently generating information to answer the item.
		  ○ Student may be writing their answer to a specific item prior to conversation about that item among group members.
		  ○ Student's written response on their worksheet may show information not present in the group conversation, suggesting independent generation of knowledge.

	Interactive (I)	• Student's contribution co-generates new information with other students or instructor/learning assistants to answer the item. Neither party shows evidence of generating the answer independently.
		  ○ If the conversation occurs between students, knowledge of more than one group member increases through this conversation.
		  ○ If the conversation occurs between a student and an instructor, the conversation results in co-generation of information for the students

		engaged in the conversation or for the entire group. • Student's statements add to information that has been previously contributed by another student. ○ Student provides new information to answer a question posed by another student. ○ Student poses a question that leads to generation of new information later in the conversation about the question. ○ The generation of new information by the first student prompts a second student to provide additional information.

Coding of Question Types

Multiple studies have investigated differences in algorithmic and conceptual questions (Nurrenbern and Pickering, 1987; Nakhleh, 1993; Zoller *et al.*, 2002; Cracolice *et al.*, 2008; Salta and Tzougraki, 2011; Surif *et al.*, 2014). However, these studies lack consistency in defining the terms "algorithmic" and "conceptual". Cracolice (Cracolice *et al.*, 2008) defined algorithmic as problems that can be solved using a memorized set of procedures, whereas Salta (Salta and Tzougraki, 2011) defined it as problems requiring students to manipulate a formula or work though an algorithm to find a numerical solution, and Surif (Surif *et al.*, 2014) defined algorithmic as "problems where all the required data, including the solution path, is known". Similar discrepancies were found with the term "conceptual". Cracolice (Cracolice *et al.*, 2008) and Nakhleh (Nakhleh, 1993) both defined conceptual as problems which require an understanding of the principles of the topic or concept where no memorized procedure or algorithm is required. Salta (Salta and Tzougraki, 2011) described conceptual as questions which "elicit student understanding of chemical ideas" by justifying a choice or making a prediction whereas Surif (Surif *et al.*, 2014) and Zoller (Zoller *et al.*, 2002) defined conceptual as questions which present an unfamiliar chemical situation which require skills such as analysis and synthesis to solve. Due to these inconsistencies, clear definitions are needed in differentiating the question types. This project used the term "algorithmic" for items where students used a set procedure or series of steps to determine the answer. Items may require algebraic manipulation of numbers to determine a numerical solution or students may need to recall or apply basic knowledge of a theory. Items were coded as "explanation" if students needed to use descriptive explanations, manipulate algebraic expressions using variables to provide conceptual explanations, or synthesize multiple pieces of knowledge together to determine an answer. For example, in the Solutions and Dilutions activity (Table 3.1), students are asked the following question: "What is the concentration when 32.74 g sucrose is used to make a 500.0 mL aqueous solution?" This question was coded as an algorithmic item since the students will mathematically manipulate the numbers given to produce a numerical result. In contrast, the following item from the same activity asked students to demonstrate their conceptual understanding of concentration and therefore was coded as an explanation item: "The images below (Figure 3.1) represent the same small volume within three different solutions and the spheres represent solute particles (solvent particles are not shown). Which solution has the lowest concentration? Circle your response and **explain** why you chose it."

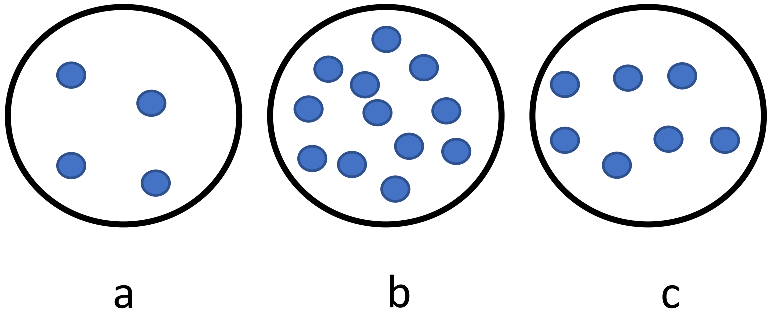

Figure 3.1: Image for explanation question example from Solutions and Dilutions activity

In this item, students must be able to define what concentration is in terms of solute particles and apply that knowledge to the images to determine which image shows the lowest concentration. They must also be able to express in words their reason for their selection.

Question vs. Group Response Coding

For each item, the question code and group response code were compared to determine if they matched. If an item was coded as Constructive/Interactive (C/I), a group response code of Constructive (C) or Interactive (I) was considered a match. In cases where the codes did not match, the group conversation was examined using thematic analysis to identify phrases which could explain the causes of the mismatch. Common causes were then combined into themes (Hsieh and Shannon, 2005; Braun and Clarke, 2020).

Factors Contributing to Individual Engagement

Using the codebook for individual engagement, codes were assigned to each student in a group for each item in the activity worksheet for each activity the student participated in. For students who participated in more than one activity during the term, for each activity, the number of codes for each ICAP category was summed, and the distribution of each student's engagement codes for each activity was determined. The trends in these distributions across multiple activities were then analyzed. In addition, trends in engagement based on group size were explored. For each activity, engagement codes were assigned to each item for each student in the group. The number of codes for each ICAP category were summed, and trends in the distribution of codes across different group sizes were observed. Conversation excerpts and interview data were used to provide support for the observed trends.

To investigate the relation between engagement and question type, once each question has been identified as an algorithmic or explanation item, a 2 x 2 contingency table was used to analyze the relation between question type and Constructive or Interactive engagement of each individual student's response to each item in the activity worksheets (Figure 3.1).

	Algorithmic	**Explanation**
Constructive		
Interactive		

Figure 3.2: Contingency table to compare student engagement with question type

At the Passive and Active engagement modes, no generation of new information occurs; therefore, these modes were not included in the analysis of the relation between engagement and question type. Because the difference between Constructive and

Interactive engagement is based on whether the generation of new information occurs through dialogue, analysis of the relation between these higher modes of engagement and question type can give insight into how different question types affect dialogue among group members. Contingency tables provide a method to statistically determine if a significant relation exists between two categorical variables (e.g., Constructive/Interactive engagement and calculation/explanation question type). These two categorical variables are not completely independent because each student is represented multiple times in the dataset since they answered multiple items in the worksheets. Therefore, McNemar's test was used to determine if a statistically significant relation exists. McNemar's test is a test to determine if a statistically significant difference exists between paired categorical data. The variables have a statistically significant relation if $p < 0.05$. If a significant relation was established, thematic analysis was applied to group responses to determine possible reasons for the relation.

Activity Structure

Recordings of student groups were also used to evaluate the effectiveness of activity worksheets on student learning in a Physical Chemistry class. The recordings of group work were analyzed using cognitive load theory to determine which items created struggle or confusion among students. The principles of scaffolding were then applied to modify these items where scaffolding is the idea of breaking down complex ideas into simpler parts (Wood *et al.*, 1976). The modified worksheets were implemented the following year and group work was again recorded. The group work using the modified worksheets was evaluated, and the effectiveness of the modified worksheets was determined.

Trustworthiness

In order to have a high level of confidence in the results of this study, its trustworthiness must be established. This can be done by evaluating the transferability, dependability, confirmability, and credibility of the work (Lincoln and Guba, 1985; Suter, 2012). Trustworthiness in this study was primarily established through credibility and confirmability.

Credibility provides evidence that the analysis of the data is an accurate representation of what actually occurred. This was established through both investigator and data triangulation. Investigator triangulation uses multiple researchers analyzing the same data whereas data triangulation uses multiple data sources for analysis, e.g., group recordings and interviews. Identification of themes which explained the mismatch in engagement codes between questions and group responses was determined by two different researchers. The researchers then discussed differences and came to consensus on the final themes.

Credibility of the individual codes was also established by investigator triangulation. Two researchers worked together to analyze conversation excerpts to identify engagement codes and develop and revise the codebook iteratively until no further revisions were needed based on transcripts. Data triangulation was established by applying thematic analysis to interview data to identify excerpts which provide additional support of the possible causes behind the observed trends in group size.

Confirmability refers to the neutrality of the researcher's analysis. When multiple researchers code text, researcher bias is minimized if agreement between the coders is high. This can be determined by calculating the inter-coder reliability (ICR) (O'Connor and Joffe, 2020). Although multiple measures of ICR exist, this project employed the commonly used Cohen's kappa (κ), a statistical measure of agreement which includes a correction for chance agreement (Cohen, 1960). Coding of a group recording of a single activity which included question, group response, and individual level was completed separately by two researchers. The researchers discussed differences in coding, modified the codebook as needed, and iteratively coded the activity until consensus was reached. The codebook was then applied by both researchers to all remaining recordings, and Cohen's κ was determined. Values of greater than 0.8 are generally considered to be a measure of good reliability (Landis and Koch, 1977).

Chapter 4: Investigating Small-Group Cognitive Engagement in General Chemistry Learning Activities Using Qualitative Content Analysis and the ICAP Framework

El-Mansy S. Y., Barbera J., and Hartig A. J., (2022), Investigating small-group cognitive engagement in general chemistry learning activities using qualitative content analysis and the ICAP framework. *Chem. Educ. Res. Pract.*, **23**(2), 335–347.

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El-Mansy collected and analyzed data, wrote manuscript; Barbera designed experiment, revised manuscript; Hartig analyzed data, wrote and revised manuscript.

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https://pdxscholar.library.pdx.edu/chem_fac/432/

Abstract

The level of students' engagement during active learning activities conducted in small groups is important to understanding the effectiveness of these activities. The Interactive-Constructive-Active-Passive (ICAP) framework is a way to determine the cognitive engagement of these groups by analyzing the conversations that occur while student groups work on an activity. This study used qualitative content analysis and ICAP to investigate cognitive engagement during group activities in a General Chemistry course at the question level, a finer grain size than previously studied. The analysis determined the expected engagement based on question design and the observed engagement based on group conversations. Comparisons of expected and observed engagement showed cases of mismatch, and further analysis determined that incorrect model use, unfamiliar scientific vocabulary, and difficulty moving between molecular representations were all contributing themes to the observed mismatches. The implications of these findings with regard to teaching and research are discussed.

Introduction

Active learning (AL) strategies have been shown to enhance student success beyond traditional methods (Kuh *et al.*, 2005; National Research Council, 2012; Freeman *et al.*, 2014), often improving outcomes for students who have been historically underrepresented within science, technology, engineering, and mathematics (STEM) fields (Lorenzo *et al.*, 2006; Haak *et al.*, 2011; Eddy and Hogan, 2014). For these reasons, AL strategies have been at the center of national calls for the adoption of evidence-based instructional practices to transform education in STEM fields (National

Research Council, 2012; President's Council of Advisors on Science and Technology (PCAST), 2012).

At the same time, evidence supporting the effectiveness of a given strategy can be inconsistent (Andrews *et al.*, 2011) and simply adding AL strategies to a learning environment does not necessarily lead to the same performance outcomes across groups (Shortlidge *et al.*, 2019). Likewise, a 2019 meta-analysis of peer-reviewed studies on the effectiveness of a wide range of AL strategies within chemistry found that the effect size of these practices varied widely, in some cases resulting in no positive impact (Rahman and Lewis, 2020). As Cooper (Cooper, 2016) points out, the umbrella of AL also covers a wide range of classroom practices, making it difficult to define what specific aspects of AL are effective and under what conditions such strategies work.

At a minimum, the effectiveness of any AL strategy depends on learners' meaningful cognitive engagement with the learning materials (Bonwell and Eison, 1991). While there is little dispute that learners benefit more from active compared to passive learning (Freeman *et al.*, 2014), a broader hierarchy of cognitive engagement has been proposed (Chi, 2009; Chi and Wylie, 2014). The ICAP framework (Chi, 2009; Chi and Wylie, 2014) offers a way to understand the varied outcomes in AL through a hierarchy of four levels of cognitive engagement: Interactive, Constructive, Active, and Passive. In this framework, simply being Active is one of the lower levels of engagement and is less likely to foster students' understanding than the higher level Constructive or Interactive modes (Chi and Wylie, 2014). In the ICAP framework, students' level of cognitive engagement is evaluated based on their overt physical and verbal behaviors (Figure 4.1). For example, behaviors related to receiving information, such as reading a text or listening to instructions would indicate Passive engagement. Active engagement would involve physical manipulations of information while learning, such as highlighting or underlining text. During Constructive engagement, students would perform the same physical manipulations that occur in Active engagement; in addition, they would generate output beyond the information provided in the learning materials. Examples of Constructive engagement include summarizing a text or taking notes in one's own words. Similar to the Constructive mode, during Interactive engagement, students would generate new information; however, this generation would occur through dialoguing among students or between students and instructors.

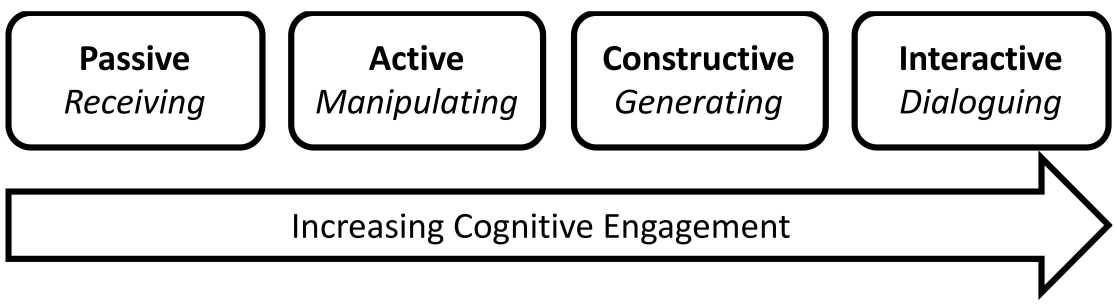

Figure 4.1: Modes of cognitive engagement (in bold) and characteristic behavior (in italics) according to the ICAP framework (Chi et al., 2018)

Studies within the ICAP framework have operationalized cognitive engagement by observing students' physical behaviors (Villalta-Cerdas and Sandi-Urena, 2014; Wiggins *et al.*, 2017), categorizing activities by their broad instructional design features (Wiggins *et al.*, 2017; Henderson, 2019; Lim *et al.*, 2019; Menekse and Chi, 2019), and analyzing student conversations (Chi, 2009; Menekse and Chi, 2019; Liyanage *et al.*, 2021). Each of these approaches has strengths and weaknesses. ICAP studies that examine engagement in terms of students' physical behaviors have used large-scale observation of overt behaviors at regular intervals at a distance in order to capture whole-class data (i.e., an observer seated in the back of the room with a chart, such as the "live coding" used by Wiggins et al. (Wiggins *et al.*, 2017) or the observation procedures used in Villalta-Cerdas & Sandi-Urena (Villalta-Cerdas and Sandi-Urena, 2014)). While this approach may be able to distinguish Passive engagement from higher ICAP levels, the differences between Active, Constructive, and Interactive engagement are difficult to tease out at this level of granularity. For example, if a student is writing something on a worksheet, this could be simply Active engagement if it involves identifying relevant information on a graph and recording the answer. However, if the student is making inferences based on trends observed in the same graph, this student would be engaging at a Constructive level. What students are saying while engaging in these physical behaviors is essential to determining what level of engagement they reflect.

ICAP studies that rely on the instructional design features of the activity as a whole are based on the idea that the structure of the activity itself will constrain the ways that students can engage with it. For example, to assess the impact of cognitive engagement on learning, Henderson (Henderson, 2019) used a series of instructional conditions designed to reflect various ICAP levels, in which a lecture-based condition was used for Passive engagement, an individual writing activity was used to elicit Constructive engagement, and a peer instruction format was used to prompt Interactive engagement. This focus on coding engagement based on instructional design features assumes, however, that all students in a group will engage at the same level throughout an activity and does not distinguish among the levels of cognitive engagement required for different types of questions or phases within an activity.

These assumptions merit greater scrutiny. Research has shown that the type of activity students participate in can affect the nature of their conversation when working in small groups (Young and Talanquer, 2013). These differences in group conversations may reflect different modes of engagement. A study on small group activities using Peer-Led Guided Inquiry (PLGI) found that students' construction of arguments varied based on the number of students participating (Kulatunga *et al.*, 2013). It is possible that these students were engaging at different levels. Variations in conversation may also be important in Process-Oriented Guided Inquiry Learning (POGIL) activities (Farrell *et al.*, 1999; Hanson *et al.*, 2018). Through the lens of the ICAP framework, not every part of an activity may elicit the same level of cognitive engagement. For example, POGIL activities involve a three-step learning cycle (Atkin and Karplus, 1962) where students first explore information provided in a model, then identify trends and patterns during the concept invention step, and finally apply the learned concept to new situations (Hanson *et al.*, 2018). The direct questions about a model during the exploration stage of this cycle are meant to ensure that students understand the model on which later parts of the activity are based. In terms of the ICAP framework, many of these questions rely primarily on Active engagement because they ask students to identify and/or reflect on information in a model that is provided for them and do not require the generation of additional information. By contrast, questions from the concept invention and application stages are more likely to elicit Constructive or Interactive engagement because they require students to make inferences that go beyond the information provided in the original model. This type of variation might be expected in any type of scaffolded learning activity.

ICAP studies that examine student conversations have generally used discourse analysis as a means for understanding student engagement during AL activities. Discourse analysis examines texts and talk in context in order to understand participants' actions (Wood and Kroger, 2000), and in education research, discourse analysis focuses on the role of spoken language in teaching and learning (Cole *et al.*, 2014). Discourse analysis research in chemistry education research has largely focused on patterns of interaction or argumentation in various instructional settings (Kulatunga *et al.*, 2013; Xu and Talanquer, 2013; Young and Talanquer, 2013; Warfa *et al.*, 2014; Current and Kowalske, 2016; Moon *et al.*, 2016; Repice *et al.*, 2016; Shultz and Li, 2016; Stanford *et al.*, 2016; Dohrn and Dohn, 2018). The use of discourse analysis in ICAP studies both within and outside of chemistry education research has generally been oriented toward the coding of individual student conversational turns; for example, the frequency of specific discourse moves (e.g., claim, accept, oppose) (Menekse and Chi, 2019), or the frequency, distribution, and engagement level evident in student conversational turns during small-group discussions (Liyanage *et al.*, 2021).

Discourse analysis can also be applied at a broader level, beyond individual turns. Because the highest two engagement levels outlined in the ICAP theory rely on distinctions that relate not just to what individual students are doing but to how they respond to one another during small-group conversations, coding longer exchanges is especially useful for distinguishing between Constructive and Interactive engagement. As noted above, there is a need to examine the extent to which actual student engagement in an activity matches the planned level of engagement based on the instructional design features of the activity itself. Therefore, using these ICAP levels as coding categories for both the activity design features and for students' observed engagement as evident in their conversations across different parts of an activity can provide a systematic way of investigating this alignment.

Whereas discourse analysis is useful in understanding *how* students interact with one another, an alternative method is needed to investigate *what* is being said, i.e., the content of the conversation. Qualitative content analysis (QCA) is well suited to filling this gap. QCA offers a method for systematically coding the content of textual data, whether verbal or written, to identify patterns (Schreier, 2012). QCA includes both deductive approaches (directed content analysis) and inductive approaches (conventional content analysis) (Hsieh and Shannon, 2005). Conventional content analysis can provide insights into phenomena that are not yet well described (Hsieh and Shannon, 2005). Because little research to date has explored the alignment between the instructional design features of individual parts of an activity and the actual level of engagement that they generate, an inductive approach is better suited to developing an understanding of instances where mismatches occur. Where mismatches between the planned and actual levels of engagement are found, conventional content analysis can be used to examine the content of students' discussions during these parts of an activity in order to identify patterns or themes that explain these mismatches. Therefore, conventional content analysis can be used to identify patterns as to which specific aspects of question design seem to foster higher or lower engagement across different groups as well as any other relevant themes that arise in students' conversations.

Research Questions

The purpose of this study is to investigate cognitive engagement during small-group activities at the question level. To do so, we used qualitative content analysis and the ICAP framework to answer the following research questions.

1. What range of engagement modes are expected during a general chemistry AL activity based on the question design?
2. What range of engagement modes are observed during a general chemistry AL activity based on students' physical and verbal behaviors during group conversations?
3. If mismatches occur between the expected and observed levels of cognitive engagement, what themes account for this mismatch?

Methods

Setting

Students from the first and second terms of a three-term General Chemistry sequence at Portland State University in the Pacific Northwest of the United States participated in this study. This course consisted of 20-30 students who were enrolled in the Honors College. Students in these courses come from a variety of STEM majors, including biology, chemistry, physics, and the pre-professional tracks, such as pre-medical and pre-dental. The first term occurred during fall quarter 2020, the second term occurred during winter quarter 2021, and the fall and winter term courses were taught by two different instructors. Classes met three times per week for 65 minutes and were conducted remotely through Zoom due to the COVID-19 pandemic. Each activity day began with a short lecture introducing the new material. Students were then placed in groups of 3-4 students in breakout rooms to work collaboratively on an activity worksheet. These groups remained consistent over the course of the term.

Activity worksheets were developed in house and structured using a format which included a model containing conceptual material followed by key questions, exercises, and problems. Key questions (KQ) generally asked about information explicitly presented in the model, providing an opportunity for students to gain familiarity with the content. Exercises (EX) included questions which required students to apply the content and infer an answer either conceptually or by performing a calculation. Problems (P) were similar to exercises but tended to be more complex, generally involving multiple steps or novel applications of the model content. The completed activity worksheets were turned in through the learning management system, and a nominal number of points were awarded for participation and attendance during the activity.

Data Collection

Institutional Review Board (IRB) approval for this research study was received from Portland State University (HRRP# 2007004-18). Students were recruited at the beginning of each term by author S.Y.E. During the fall term, seven students consented to participate and were divided into two groups: Group A consisted of four students and Group B consisted of three students (Table 4.1). Three students from the fall also consented to participate during winter term and formed a new group: Group C. All student names reported in this manuscript are pseudonyms.

Three activities were observed during fall term and one activity was observed during winter term. The activities during the fall were evenly spaced, with the first one covering the concepts of mole and molar mass occurring near the beginning of the term, the second one covering concepts involving solutions and dilutions occurring near

Table 4.1: Groupings for study

Fall 2020		**Winter 2021**
Group A	**Group B**	**Group C**
Nani	Jacob	Nani
Beth	Helen	Helen
Katie	Grace	Grace
Leslie	---	---

polarity occurring near the end of the term. During winter term, the single activity occurred near the beginning of the term and covered concepts surrounding thermal energy and calorimetry. Each breakout room session was audio and video recorded. These recordings were transcribed verbatim by a transcription service. Transcripts were then reviewed and edited as needed by author S.Y.E and pertinent physical actions from the participants (e.g., nod of agreement) were added to the transcripts. Unclear conversation was denoted by [XXX] in the transcripts.

Data Analysis

Most of the prior work done using ICAP to investigate engagement during group activities assumed a single engagement mode over an entire activity (Menekse *et al.*, 2013; Wiggins *et al.*, 2017; Henderson, 2019). As these activities may contain different types of questions, this assumption may not be correct. Therefore, for the four activities observed, a finer grain size was used. The unit of analysis was each question within an activity. At this level of analysis, each question was first coded according to the ICAP framework where the intended engagement mode of students was identified based on the question design.

Previous work investigating group conversations using ICAP looked at quantitative measures such as frequency of conversational turns or discourse moves (Wiggins *et al.*, 2017; Menekse and Chi, 2019); however, this type of analysis does not provide insight into the relation between the group conversation and the question design. To address this gap, a second round of coding applied the ICAP framework to the group responses to each question in an activity. Each group's response to a question was coded based on the content of the conversation and the definition of each of the ICAP modes. The codebook for both types of coding is presented in Table 4.2. Each question and group response in the transcripts was coded deductively based on features of the levels of engagement outlined in the ICAP framework (Chi, 2009; Chi and Wylie, 2014).

Table 4.2: Codebook for question and group response codes

Question Codes	
ACTIVE (A)	Information to answer the question can be found in the provided materials.
CONSTRUCTIVE/INTERACTIVE (C/I)	New information needs to be generated to answer the question prompt.
Group Response Codes	
ACTIVE (A)	Conversation reflects that an answer was taken from information provided.
CONSTRUCTIVE (C)	One person provides the answer, generating new information. Can include forms of agreement from other group members (e.g., head nods, "yeah", "uh-huh", etc.).
INTERACTIVE (I)	Participants generate information to answer the question based on one another's responses. Other participants' contributions of off-topic talk or forms of agreement are not included in this code.

Question Coding

Three of the four engagement modes of ICAP (Figure 4.1) were applied to each question in an activity (Table 4.2). For multi-part questions, each part was assigned a separate code. Passive engagement was not used to code questions because the questions were designed to be used in a group activity with the *intent* for students to engage actively at a minimum. Questions were coded as Active (A) if the information to answer the question could be found in the presented materials; it was assumed that students would use this information in their response. For the higher engagement modes (i.e., Constructive and Interactive), the difference between these modes is determined by whether the generation of new information occurs through dialogue. Since it is not possible to distinguish this difference based on the structure of the questions alone, Constructive and Interactive engagement were collapsed into a single code, Constructive/Interactive (C/I).

Group Response Coding

Each group response to a question (or part of a question, for multi-part problems) was coded separately, resulting in a response code for each question answered in each activity. Passive engagement was not used as a code because by virtue of conversation simply occurring, students were manipulating information, and therefore, the lowest mode of engagement students could participate in at the whole-group level would be Active. Although it is possible for *individual* students to be engaging passively, the group response code was based on the conversation that occurred among all group members. The response was coded as Active (A) if the students in a group explicitly referred to the information presented in the activity in their response. The Constructive (C) code was defined by the conversation generating new information to respond to the question; this new information was generated by a single student. Conversation may still occur between students with other students agreeing with the student generating information; however, this type of dialogue does not constitute *co*-generation of information and therefore would still be coded as Constructive. This contrasts with the Interactive (I) code where new information is generated through dialogue between two or more students. During the dialogue, each student contributed new information and each contribution built upon information previously generated in the conversation.

Mismatch between question and group response codes

Across all four activities and three groups, group responses were observed, coded, and compared to the corresponding question code. When the question code and the group response code were not the same, this was identified as an instance of mismatch. Since Constructive and Interactive engagement were a single code (i.e., C/I) for the questions, if the corresponding group response was coded as Constructive or Interactive, either of these was considered a match. For each case of mismatch, the group conversation was examined inductively using conventional content analysis (Hsieh and Shannon, 2005) to determine if there were any themes that may explain the cause of the mismatch. To identify potential causes, each question and group response showing mismatch was read by two researchers. The researchers then independently identified specific phrases which were thought to contribute to the cause of the mismatch. The researchers then discussed these mismatch causes and combined common causes into themes.

Trustworthiness

Trustworthiness of the findings in this study was established through the evaluation of quality criteria such as qualitative reliability and credibility (Korstjens and

Moser, 2018; O'Connor and Joffe, 2020). To enhance reliability in coding the questions and responses, a secondary coder was employed to evaluate the application of the codes in a two-stage process. The author S.Y.E developed the codebook (Table 2), and both author S.Y.E and the secondary coder first each individually coded each question and group response in a single activity. The coders met, discussed and resolved differences in coding, and came to consensus. Through the discussion to achieve consensus, the coders agreed that no modifications to the codebook were needed. The two coders then coded all the questions and group responses across the remaining activities. Inter-rater reliability (IRR) at each stage was evaluated by calculating Cohen's kappa (Cohen, 1960). During the first stage, the IRR values for question and group response coding of the single activity were 0.88 and 0.56, respectively. The IRR values for the subsequent question and group response coding across all remaining activities during the second stage were 1.00 and 0.99, respectively. Kappa values greater than 0.8 are generally considered to have good reliability (Landis and Koch, 1977). For the identification of themes related to mismatched engagement levels between the questions and group responses, investigator triangulation (Lincoln and Guba, 1985) was used to establish credibility. Two of the authors (S.Y.E and A.J.H) used conventional content analysis to identify patterns in the transcripts and worked together to combine these patterns into themes.

Results and Discussion

Question Coding

Questions were coded as either Active (A) or Constructive/Interactive (C/I) based on how the information to answer would be derived (Table 4.2). Figure 4.2 presents a portion of the model from the Solutions and Dilutions (SD) activity.

Excerpt of Model from Solutions and Dilutions (SD) Activity

What are stock and dilute solutions? – Often times in lab you are given a stock solution, this solution typically has a higher concentration than you will need for your experiment. In running an experiment, you typically use dilutions made from this stock solution. *Dilutions* (or dilute solutions) are solutions with lower concentrations than the stock solution.

In a dilution, an aliquot of the stock aqueous solution is diluted by adding more water. In doing this, the volume of the dilute solution increases but the number of moles of solute remains constant. As the number of moles of solute remain constant, the following equality can be made.

Relation between concentrated and dilute solutions

$M_C \times V_C = moles\ of\ solute = M_D \times V_D$	
M_C = molarity of **concentrated** solution	M_D = molarity of **dilute** solution
V_C = volume of **concentrated** solution	V_D = volume of **dilute** solution

Figure 4.2: Portion of model from Solutions and Dilutions (SD) activity

For example, Key Question 6 from the Solutions and Dilutions activity (SD-KQ6) was coded as Active because the information in the model (Figure 4.2) explicitly states the required information in the text blurb and in the equation in the gray box at the top of the table.

SD-KQ6) *When making a dilute solution, which of the following remains constant?*

i) The concentration ii) The moles of solute iii) The volume of the solution

However, Key Question 9 from the same activity (SD-KQ9) asks students to provide an algebraic expression for M_D (i.e., the molarity of the dilute solution). Since this question asks students to manipulate the equation in the model (Figure 4.2), they would be generating new information. Therefore, SD-KQ9 was coded as a Constructive/Interactive question.

SD-KQ9) *In preparing for an experiment, you need to know what the concentration of a dilute solution (M_D) will be. Provide an algebraic solution using the relation in the model for this concentration.*

In total, 68 questions were coded across the four activities (Table 4.3). Since the groups did not complete the activities in their entirety during the time allotted, the data includes only those activity questions which had a corresponding group response. Additionally, questions which were answered by both Groups A and B were counted only once. The overall results show that 13 questions were Active and 55 questions were Constructive/Interactive.

Table 4.3: Frequency of Active vs. Constructive/Interactive Question Coding by Activity. Percentage of question codes per activity are given in parentheses

Activity	Active Questions	Constructive/Interactive Questions
Mole and Molar Mass	2 (11)	16 (89)
Solutions and Dilutions	3 (23)	10 (77)
Electronegativity and Polarity	3 (17)	15 (83)
Thermal Energy and Calorimetry	5 (26)	14 (74)
Total	13 (19)	55 (81)

In general, the majority of questions (81%) were Constructive/Interactive questions across all activities. Table 4.3 shows that within the different activities, the percentage of questions coded as Active can vary, consisting of up to around one quarter of the total coded questions. Such variation was not captured in previous studies which coded at the activity level (Menekse *et al.*, 2013; Wiggins *et al.*, 2017; Henderson, 2019).

Group Response Coding

Group responses were coded as Active (A), Constructive (C), or Interactive (I) based on if more than one student contributed to the answer and whether their response(s): 1) generated new information, and 2) involved students building upon each other's statements to develop a final answer. In the conversation excerpts that follow, line numbers are used to allow for easy identification of pertinent portions of the text, information in parentheses refers to non-verbal actions, and information in square brackets has been added to the transcripts for clarity.

Excerpt 1 illustrates a group response that was coded as Active. In this excerpt, members of Group A are responding to SD-KQ6. Beth's comment (line 261) mentions looking at the equation which is a reference to the model (Figure 4.2); therefore, this group response was coded as Active.

SD-KQ6) *When making a dilute solution, which of the following remains constant?*

i) The concentration ii) The moles of solute iii) The volume of the solution

Excerpt 1: Group response to SD-KQ6, coded as Active

260 KATIE: Okay. So, key question six: "When making a dilute solution, which of the following remains constant?" Circle your response: "One, the concentration, two, the moles of the so-, solute, or three, the volume of the solution."

261 BETH: It looks from the equation [in the model] that the moles of the solute stay constant.

262 NANI: Yeah.

Excerpt 2, on the other hand, illustrates a group response that was coded as Constructive. This excerpt focuses on Group C's response to Key Question 3 from the Thermal Energy and Calorimetry activity (TEC-KQ3) where students are asked to explain the difference in heat capacity between two blocks. Figure 4.3 presents a portion of the model from the Thermal Energy and Calorimetry (TEC) activity.

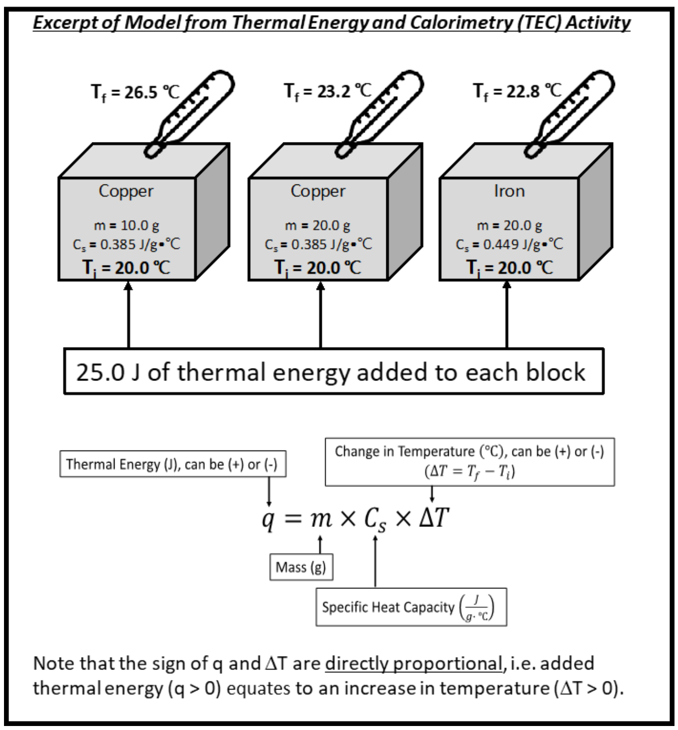

Figure 4.3: Portion of model from the Thermal Energy and Calorimetry (TEC) activity

In Excerpt 2, Helen provides the answer to the question associated with this portion of the model (lines 52), and the contributions from Nani and Grace are forms of agreement (lines 53 and 54). Therefore, Helen is the only student generating new information and this group response was coded as Constructive.

TEC-KQ3) *How does the <u>difference in specific heat capacity</u> between blocks 2 and 3 relate to their final temperature? Briefly explain.*

<u>Excerpt 2: Group response to TEC-KQ3, coded as Constructive</u>

51 GRACE: So, “How does the difference in specific heat capacity between blocks two and three relate to their final temperature?”

52 HELEN: So it, it's the same as mass, right? So, like a greater specific heat capacity will result in a lower final temperature.

53 GRACE: Yeah.

54 NANI: (nods).

55 HELEN: So, so block two will have a greater final temperature.

586 GRACE: Mm hmm.

Excerpt 3 gives an example where the coding of the group response was ambiguous. In this excerpt, students from Group A respond to Key Question 7 from the Solutions and Dilutions activity (SD-KQ7). Although the answer is present in the model (Figure 4.2), and Katie gives the correct answer (line 271), it is unclear from the conversation whether Katie’s response was based on the information in the model (Active) or she generated new knowledge (Constructive). In the absence of evidence that the response came from the model, it was assumed that she generated new knowledge and the group response was coded as Constructive.

SD-KQ7) *When making a dilute solution, which of the following* ***decreases****? Circle your response.*

i) The concentration ii) The moles of solute iii) The volume of the solution

<u>Excerpt 3: Ambiguous group response to SD-KQ7, coded as Constructive</u>

270 BETH: Okay. The sec-, or the seventh quest-, seven, seventh key question is, um, "When making a dilu-, dilute solution, which of the following decreases, circle your response? Um, one, the concentration, two, the moles of the solute, or three, the volume of solution."

271 KATIE: Wouldn't it be the concentration since we're diluting it?

272 BETH: Yeah, I think so.

Excerpt 4 shows an example of interactive engagement where Katie, Leslie, and Beth all contribute new information to solving the calculation in Exercise 5 from the Solutions and Dilutions activity (SD-EX5). Leslie and Katie start by determining what variable they are solving for (lines 400 and 401). Leslie then builds on this by identifying the numerical value for M_C, and Katie further contributes new knowledge by mentioning the form of the equation they should use to solve (lines 403 and 404). Beth further builds on this knowledge by providing the numerical solution (line 408). Since Leslie, Katie, and Beth all contribute pieces of information to answer the question and each of their statements builds upon the previous student's comment, this response was coded as Interactive.

SD-EX5) *What is the concentration when 11.75 mL of 0.375 M sucrose is diluted to 50.0 mL?*

Excerpt 4: Group response to SD-EX5, coded as Interactive

400 KATIE: Ok, "What is the concentration when 11.75 milliliters of 0.375 molarity or mole?" I don't even know. Sucrose is diluted to 50 milliliters. Okay. So now we're trying to find M_C. Again, M_C.

401 LESLIE: No, we're find-, we're trying to find, M_D now.

402 BETH: Yeah. I think M_D.

403 LESLIE: Cause M_C is that 0.375.

404 KATIE: Oh yeah, so we're finding...so we would do our M_C times V_C divided by V_D then?

405 BETH: Yeah.

406 LESLIE: Did you guys get there?

407 KATIE: Just about...Oh geez!

408 BETH: Do you guys get 0.0881?

409 LESLIE: Mm hmm.

In total, 101 group responses were coded (Table 4.4). Groups A and B have a different number of response codes for each activity because they moved at different speeds and therefore did not answer the same number of questions. As with the question coding, since students did not complete the activities during the time allotted, coded responses are only for completed questions, not all questions in the activity. Overall, group responses were distributed across the three engagement modes with 8 responses coded as Active, 32 responses coded as Constructive, and 61 responses coded as Interactive. Results indicate that Interactive group responses ranged from 64% to 87% for Group A and from 39% to 77% for Group B across the Mole and Molar Mass, Solutions and Dilutions, and Electronegativity and Polarity activities. Only Group C completed the Thermal Energy and Calorimetry activity, and only 58% of their responses during this activity reached the level of Interactive engagement. Overall, observed engagement levels across groups and across questions within an activity varied widely.

Table 4.4: Frequency of group response codes by activity and group. Percentages of group response codes by activity and group are given in parentheses

Activity	Group	Active Responses	Constructive Responses	Interactive Responses
Mole and Molar Mass	A	0 (0)	1 (13)	7 (87)
	B	1 (6)	7 (39)	10 (55)
Solutions and Dilutions	A	1 (9)	3 (27)	7 (64)
	B	1 (8)	2 (15)	10 (77)
Electronegativity and Polarity	A	0 (0)	5 (36)	9 (64)
	B	2 (11)	9 (50)	7 (39)
Thermal Energy and Calorimetry	C	3 (16)	5 (26)	11 (58)
Total		8 (8)	32 (32)	61 (60)

Matches between question and group response codes

A total of 68 questions (Table 4.3) and 101 group responses (Table 4.4) were coded across the three groups and four activities. We began the comparison between coding groups by examining the questions coded as Constructive/Interactive and their corresponding group responses. Table 4.5 shows the breakdown of the frequency of Constructive/Interactive coded questions by activity and group. It also shows how the group responses were distributed across the Constructive and Interactive codes. These results indicate that when the question was coded as Constructive/Interactive, all the group response codes were either Constructive or Interactive, indicating a match with this question code but different levels of engagement. Across all groups and activities, the portion of group responses coded as Interactive ranged from 40% to 90%. In total, just over two-thirds of the responses were coded at the level of Interactive engagement.

Table 4.5: Breakdown of frequency of Constructive and Interactive question and group response codes by activity and group. Percentages of Constructive and Interactive group responses are given in parentheses

Activity	**Group**	**Constructive/Interactive Question Codes**	**Constructive Group Response Codes**	**Interactive Group Response Codes**
Mole and Molar Mass	A	8	1 (13)	7 (87)
	B	16	7 (44)	9 (56)
Solutions/Dilutions	A	8	1 (13)	7 (87)
	B	10	1 (10)	9 (90)
Electronegativity/Polarity	A	11	4 (36)	7 (64)
	B	15	9 (60)	6 (40)
Thermal Energy/Calorimetry	C	14	5 (36)	9 (64)
Total		82	27 (33)	55 (67)

In addition to variation in response coding seen across activities, variation was also observed across groups (Table 4.6). For groups A and B, who completed the same three activities, several of the response codes differed across the two groups on the questions that both groups completed. For example, Table 4.6 shows that on the 8 completed questions coded as Constructive/Interactive in the Mole and Molar Mass activity, the responses of groups A and B only overlapped on 6 question responses, all coded as Interactive. The fewest matches between groups were observed on the 11 Electronegativity and Polarity questions, with only 5 of the response codes matching.

Table 4.6: Distribution of response matches between Groups A and B across the Constructive/Interactive questions that were answered by both groups

Activity	**Constructive/Interactive Questions Answered by Both Groups**	**Constructive Group Response Matches**	**Interactive Group Response Matches**
Mole and Molar Mass	8	0	6
Solutions/Dilutions	8	1	5
Electronegativity/Polarity	11	2	3

Upon comparison of question codes to the response codes of each group, mismatches were found exclusively in questions coded as Active. A breakdown of the frequency of questions and group responses coded as Active is shown in Table 4.7. While 19 total questions were coded as Active, only 8 responses were also coded as Active, a 42% match. This means that more than half of the questions coded as Active had a mismatch with their corresponding group response codes, where students were responding at a higher engagement mode than was indicated by the question design. Among the 11 Active questions which showed a higher group response engagement mode, the responses split almost evenly between Constructive (5) and Interactive (6) engagement.

To further investigate these mismatches, conventional content analysis was used to identify the potential causes by examining each mismatched question and group response for specific phrases that identified the source of the mismatch. Causes were then collected into common themes. Table 4.8 summarizes these results. Each of the questions in these mismatched cases was coded as Active because the information to answer the question was explicitly available in the activity.

Table 4.7: Breakdown of frequency of Active question and corresponding group response codes by activity and group

Activity	Group	Active Question Codes	Active Response Codes	Constructive Response Codes	Interactive Response Codes
Mole and Molar Mass[a]	A	0	0	0	0
	B	2	1	1	0
Solutions/Dilutions	A	3	1	2	0
	B	3	1	1	1
Electronegativity/Polarity	A	3	0	1	2
	B	3	2	0	1
Thermal Energy/Calorimetry	C	5	3	0	2
Total		19	8	5	6

[a] Groups A and B have different numbers of Active questions because Key Questions 1-4 were assigned prior to class, and Group A did not discuss them while Group B went over them as a group before proceeding.

Table 4.8: Frequency of mismatched question and response codes with associated themes

Theme	Activity	Group	Mismatched Cases
Model Use	Thermal Energy/Calorimetry	C	2
	Mole and Molar Mass	B	1
Unfamiliar Vocabulary	Solutions/Dilutions[a]	A	1
		B	1
Molecular Representations	Electronegativity/Polarity[a]	A	2
		B	1
Ambiguous	Solutions/Dilutions[a]	A	1
		B	1
	Electronegativity/Polarity	A	1

[a] The mismatched cases in these activities occurred on the same questions in Groups A and B.

Themes relating to mismatch

Conventional content analysis was used to investigate each of the group responses for details that explain the higher level of engagement displayed by the conversation compared to the question. The analysis suggested three possible themes: model use, unfamiliar vocabulary, and molecular representations. Although Key Question 7 from the Solutions and Dilutions activity (SD-KQ7) and Key Question 4 from the Electronegativity and Polarity activity (EP-KQ4) showed a mismatch, our inductive analysis did not suggest that the cause of mismatch in these cases falls into one of the identified themes. The group responses on these items were deemed to be ambiguous because it was not clear from the conversation if the students' response was taken from the activity material.

Theme 1: Model Use

Three of the 11 instances of mismatch were due to improper model use. These cases occurred during the Thermal Energy and Calorimetry (TEC) and the Mole and Molar Mass (MM) activities. Because the answers to these questions were explicitly stated in the model, it was expected that the students would use the model to answer these questions, and that the group conversation would show evidence of this.

For example, in Excerpt 5, Group C responds to Key Questions 4 and 5 from the Thermal Energy and Calorimetry activity (TEC-KQ4 and TEC-KQ5). Since the answers to both these questions are explicitly stated in the model (Figure 4.3), these questions are coded as Active. Although the group response to TEC-KQ4 did refer to the model and was coded as Active, the response was incomplete. The correct response should have included ΔT and q, but Helen and Grace used the model to decide that the answer should only include ΔT (lines 68-71). Because of this incomplete use of the model, Helen and Grace engaged interactively to answer the next question in the activity, TEC-KQ5, which built upon the aspects of the model highlighted in TEC-KQ4. This interaction starts from line 72 and Grace's realization that they need two variables. From there, Helen builds upon this, suggesting the two variables are T_i and T_f (line 73). Although the final answer they come to is incorrect, one can see that it is the incomplete use of the model in TEC-KQ4 which prompts the interactive engagement in TEC-KQ5.

TEC-KQ4: *When mathematically determining q, which variables can be positive or negative?*

TEC-KQ5: *How are the two variables in KQ4 related?*

Excerpt 5: Example of incomplete model use

68 GRACE: It s-, it shows at the top model [referring to the model in Box 2], which ones. So...

69 HELEN: Yeah, it does. So only ΔT.

70 GRACE: Yeah. ΔT, and if you want to include the thermal energy, you could say that, but we're already talking about it, so...

71 HELEN: Yeah. I don't think you would include q.

72 GRACE: And then, "How are the two variables related?" Um...Oh, they said the two variables. Okay. So, you can't include q. It's the same thing...

73 HELEN: Okay. No, no. So, it's temperature final and temperature initial.

74 GRACE: Oh, those are the two variables. Ohhh...

75 HELEN: Yeah.

76 GRACE: Okay. Never mind. Um, But the temp...Oh yeah. The temp can be negative.

77 GRACE: Well If one's, if one's, it depends on which one, if the final's higher than the initial, then you get a positive number. If the initial's higher than the final, you get a negative number. So I suppose that's how it's related...right.

Theme 2: Unfamiliar Vocabulary

Two of the 11 instances of mismatch involved students' use of unfamiliar vocabulary, specifically the scientific term "aliquot" in Key Question 8 of the Solutions and Dilutions activity (SD-KQ8). Although this question is coded as Active because the information to answer the question is explicit in the model (Figure 4.2), responses from both Groups A and B display a higher mode of engagement due to unfamiliarity with the term "aliquot". For example, in Excerpt 6, the higher engagement mode of Group B's response is prompted by Helen's question about the meaning of "aliquot." Jacob responds and Grace looks up the definition ostensibly on Google (lines 166-168). It is evident that the interactive engagement resulted from unfamiliarity with the term "aliquot".

SD-KQ8) *In a dilution, which is always* ***larger****? Circle your response.*

i) The volume of the aliquot ii) The volume of the final solution

Excerpt 6: Example of unfamiliar vocabulary

166 HELEN: I know it's the second one, but what exactly is the ali- aliquot? Cause I know [XXX] fairly small, so small sample or whatever.

167 JACOB: I guess the aliquot would be, do you think it would be the given volume?

168 GRACE: I'm just looking it up.

169 JACOB: Fair enough.

170 HELEN: What does Google say?

171 GRACE: A portion of a larger whole, a specific sample taken for chemical analysis or other treatment. I think it's like a portion of the sample. So the portion is obviously going to have less.

172 JACOB: So in a dilution, which is yeah, the volume of final solution will be larger.

Theme 3: Molecular Representations

Communicating complex scientific ideas is dependent on using multiple "languages of science", which may include symbolic, graphical, or mathematical representations (Osborne, 2010). Four of the 11 instances of mismatch involved students' struggles in moving between different representations in the Electronegativity and Polarity activity. Figure 4.4 depicts a portion of the model from this activity. Key Question 8 from the Electronegativity and Polarity activity (EP-KQ8) asks students to explain why DL_2 is a polar molecule. Since this information is depicted in the model (Figure 4.4), this question is coded as Active. Students in Groups A and B seemed to have difficulty moving between the Lewis structure representation and bond dipole representation of molecules. In Excerpt 7, the Interactive engagement of Group A is

Excerpt of Model from Electronegativity and Polarity (EP) Activity

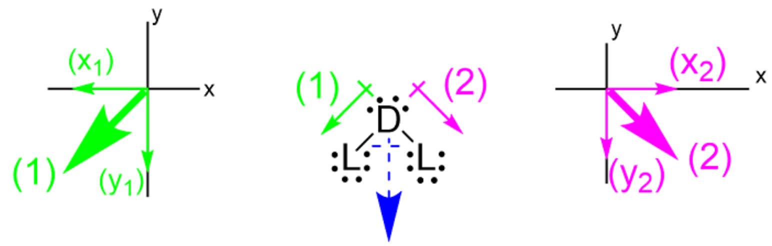

Figure 5: Bond dipole moments 1 and 2 are divided into their x- and y-components x_1, y_1, x_2, and y_2. The x-components (x_1 and x_2) point in opposite directions and cancel out. The y-components (y_1 and y_2) point in the same direction, adding together to give the resultant molecular dipole.

Figure 4.4: Portion of model from the Electronegativity and Polarity (EP) activity

prompted by Beth asking about the number of arrows that should be drawn (line 285). Leslie builds on the question explaining that she drew three arrows (line 286), and the instructor (INST in excerpt) builds further adding new information that there should be two component arrows for each bond dipole (line 290).

EP-KQ8: *Using the blank Cartesian coordinate system, draw the x- and y-components of each bond and use them to explain why DL_2 is a polar molecule.*

Excerpt 7: Example of molecular representations (Group A)

285 BETH: For this one, do you only draw two arrows or should there be more than two?

286 LESLIE: I'm doing three for that one. So like the two going on the X and then the one going down for the Y.

287 BETH: OK.

288 INST: [Key Question] Eight. Okay. And are you looking at it or have you talked about it?

289 BETH: Um, we've talked about how many arrows to draw and um, I think we decided on drawing like three arrows. Uh, I drew like two, um, on the X axis like going different directions and then one down on the Y axis.

290 INST: Okay. So for each of the diagonal arrows, they have both an X and a Y component. Yeah. So the downward, yes. I see what, you're what you're drawing, Katie. So you, so you have for each of the diagonals, you have an X and a Y. And so for this one, you have an X and a Y. So you actually have two downward arrows on the Y axis.

291 BETH: Two downwards? Ok.

While the Interactive engagement in Excerpt 7 was prompted by difficulty in translating between the Lewis structure and the representation depicting bond dipoles, in Except 8, we see a desire to understand more deeply the role of specific features of the Lewis structure (i.e., lone pairs of electrons) in the dipole representation is the trigger for the Interactive engagement. In Excerpt 8, Group B engages interactively to try to gain a deeper understanding of what the vector model of dipoles represents. Their response to the same question begins with a discussion of the Lewis structure to identify the molecular geometry (lines 368-371). From there, they reference the model to determine how to draw the components of the bond dipoles (lines 373-386). Lines 387-396 show the group generating new information as they attempt to make the connection between the lone pairs of electrons in the Lewis structure and the bond dipoles. In lines 385 and 386, both Helen and Jacob directly refer to Figure 4.4 in the model, stating that the answer is there (Active engagement). However, Grace's desire to understand how the lone pairs fit into the vector representation causes the group to engage at the higher Interactive mode (lines 387 and 393). In both groups' conversations, it is apparent that the students attempting to move from the Lewis structure representation of the molecule to the vector model of bond dipoles is the trigger for the higher mode of engagement.

<u>Excerpt 8: Example of molecular representations (Group B)</u>

368 GRACE: Oh, and this one has lone pairs. What kind of structure does that make?

369 JACOB: The chart's...DL2, lone pairs.

370 JACOB: It's bent.

371 GRACE: I think bent?

372 JACOB: Yeah.

373 JACOB: Cause if we're looking at the model, um, the model gives like the best description of it above, uh, for the DL2. So net molecular

dipole due to bent geometry. And it shows you below what that bent geometry looks like on the planes.

374 GRACE: So for this we're doing four.

375 JACOB: And it's asking us why it's polar.

376 GRACE: Oh, I'm assuming they don't cancel each other out.

377 HELEN: The left and right aspects do, but they still have a net, like, down.

378 GRACE: Wait, what?

379 JACOB: It has a net molecular dipole.

380 GRACE: Yeah. No...Have you guys started drawing the coordinate? I don't know how they'll look. Are they pointing down Y?

381 JACOB: They're pointing down, yeah, Y.

382 GRACE: Okay. At what angle?

383 HELEN: Like 45ish each in the third and fourth quadrant.

384 JACOB: Like it's coming out of the origin.

385 HELEN: I mean, it's just like the green and pink arrows in Figure 4 is what I drew. But on one axis or like one....

386 JACOB: Same. I simply, I literally don't know why, like I know, but I also like don't know, so I just looked at Figure 4 that has the answer so... Well, it has what we're supposed to be gathering from it.

387 GRACE: What about the lone pairs?

388 JACOB: Um, it shows in Figure 4, like kind of, uh, the lone pairs are kind of like on the arrows or like, do you see Figure 4?

389 GRACE: Oh yeah.

390 JACOB: So that's kind of what Figure 4 does with the...

391 GRACE: So I've got two of them with the arrows pointing opposite ways in the third and fourth quadrants.

392 JACOB: Yes.

393 GRACE: What are the ones for the lone pairs?

394 HELEN: It just says of each bond. I don't think you have to worry about the lone pairs.

395 JACOB: And then ask why it's polar. And um, like Helen said, it doesn't cancel because of the net molecular dipole.

396 HELEN: I said it's polar because though the dipoles cancel out in the x-direction, they have a net downward dipole moment. I don't think that's like correct language, but...

397 JACOB: I mean, I think it's it, but it gets your point across.

Conclusion

Previous studies using the ICAP framework of cognitive engagement to investigate active learning environments assumed a single engagement mode for the entire activity (Wiggins *et al.*, 2017; Henderson, 2019). However, the data examined above suggest that students may engage differently with different parts of an activity. In addition, some studies have also assumed an engagement mode based on the activity design instead of overt student behavior (Menekse *et al.*, 2013; Wiggins *et al.*, 2017). ICAP identifies engagement modes based on student behavior, and as seen above, it may not be accurate to assume the expected engagement mode based on activity design would be the same as the observed engagement mode based on student behaviors. To address these concerns, we used ICAP to investigate cognitive engagement of student groups during AL activities in answering the following research questions.

RQ1: What range of engagement modes are expected during a general chemistry AL activity based on the question design?

This study used a finer grain size, i.e., identifying engagement modes at the question level rather than the activity level. Results indicated that across the four activities observed, the majority of questions (81%) were designed to elicit Constructive or Interactive engagement. Investigation at this finer grain size confirms that not all questions were designed with the same mode of engagement in mind, and therefore studies which assume a single engagement mode for the entire activity may miss insights that can be seen when looking at engagement at the question level.

RQ2: What range of engagement modes are observed during a general chemistry AL activity based on students' physical and verbal behaviors during group conversations?

The study also identified observed engagement modes of student groups by using ICAP to examine group conversations. Results indicated that within a single activity, the engagement of the group based on their conversation varied from Active to Interactive, with the majority of the group responses (60%) showing Interactive engagement. Additionally, within each group, the percentage of Interactive responses was not consistent across all activities (64%-88% for Group A; 39%-77% for Group B). These results provide further evidence that coding engagement at the question level for both questions and responses can give insight into students' engagement which is lost when coding at the activity level.

RQ3: If mismatches occur between the expected and observed levels of cognitive engagement, what themes account for this mismatch?

By comparing the expected engagement mode based on the question design with the observed engagement mode based on the group responses, cases of mismatch were identified. The group conversations were then further investigated using qualitative content analysis for common themes that caused the mismatches. Results suggested that the causes of the higher than expected observed engagement levels were related to three themes: model use, unfamiliar vocabulary, and struggles with different molecular representations.

Limitations

Due to the small sample size used in this study, these results are not generalizable to large populations. Additional studies are being conducted in author Barbera's research group to provide more generalizable insights into students' engagement in small group learning activities. Since the observed groups were recorded through Zoom, we were unable to see what students were writing unless papers were held up to the camera. Because of this limitation, engagement modes of groups were based solely on the group conversation. However, being able to see what students were writing on their worksheets could have provided additional insight into their cognitive engagement. Future data collections will take place in person and will be able to account for these actions. Finally, the coding of activity questions according to ICAP was based solely on design features present in each question and not explicitly on any stated intention on the part of the activity designers. Therefore, although the activity questions may have been written to elicit a specific type of thinking or engagement on the part of the students, the questions could only be coded based on specific features that were present in the questions themselves.

Implications for Instructors

Results of this study showed that there were multiple instances of Constructive or Interactive engagement occurring in Key Questions where Active engagement was expected. Incomplete or lack of model use was one reason for this. In some cases, this resulted in students engaging at a higher level but obtaining an incorrect answer. While many instructors discuss the structure of and expectations for these types of learning activities at the start of a term, we would suggest that instructors regularly remind students to read through the model prior to answering any questions in the worksheet and to refer back to it in their responses. This would reinforce the purpose of the models and may focus the groups' conversations on the data and details within the materials.

Use of new and potentially unfamiliar scientific terms can possibly promote students' curiosity and potentially lead to higher modes of engagement. This idea was supported in this study where use of the unfamiliar term "aliquot" resulted in more conversation and a higher engagement mode. Although there is the danger that discussion of such vocabulary could result in unhelpful, tangential conversations, group discussions around the term “aliquot” seemed to help students reason out an answer to the question. In addition, learning relevant new vocabulary is essential to students’ growth as scientists. Therefore, use of unfamiliar vocabulary that is relevant to the concept being taught can be a useful tool to promote student learning.

It should be noted that although ICAP states that cognitive engagement increases as one moves from Passive to Active to Constructive to Interactive, it should not be inferred that Interactive engagement is always the most desirable. As shown in this study, these higher than expected modes were due to a variety of factors that could provide insight to future improvements in the activities or instructional practices. Worksheets for these activities were structured such that students begin with Key Questions which are designed to orient students to the pertinent information in the model (i.e., Active engagement), followed by Exercises and Problems, which allow students to manipulate and apply the information in a more advanced manner (i.e., Constructive or Interactive engagement). By scaffolding worksheets in such a manner, students use knowledge gained at the lower engagement modes to foster a deeper understanding during the more complex Exercises and Problems.

Implications for Research

Investigation of student conversations using qualitative content analysis has opened avenues of further exploration. While this study looked at the engagement mode of the group as a whole, it is apparent that not all participants within a group are engaging to the same degree. For example, in Group A, Nani was a very quiet student who rarely contributed to conversations but was always writing on her worksheet and nodding along with other students' statements. Exploring the individual students' engagement could provide insight into how a student's engagement correlates with learning outcomes. Other factors such as group dynamics and how these dynamics change over time may also be understood by analyzing the engagement of each individual. In addition, further exploration into the root causes of the identified mismatch themes can be explored. For example, the unfamiliar vocabulary theme could be due to differences in prior knowledge that students bring to the activity. Research in this area could increase understanding of how prior knowledge affects students' engagement in small-group activities.

Conflicts of Interest

There are no conflicts of interest to declare.

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Chapter 5: Factors Affecting Individuals' Cognitive Engagement during Group Work in General Chemistry: Timing, Group Size, and Question Type

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El-Mansy collected and analyzed data, developed codebook, wrote manuscript; Stephens provided secondary coding for question type items; Mortensen developed codebook; Francis developed codebook; Feldman developed codebook; Sahnow reviewed and cleaned transcripts; Barbera revised manuscript; Hartig analyzed data, developed codebook, revised manuscript.

Abstract

Understanding how individual students cognitively engage while participating in small group activities in a General Chemistry class can provide insight into what factors may be influencing their level of engagement. The Interactive-Constructive-Active-Passive (ICAP) framework was used to identify individual students' level of engagement on items in multiple activities during a General Chemistry course. The effects of timing, group size, and question type on engagement were investigated. Results indicate students' engagement varied more in the first half of the term and students demonstrated higher levels of engagement when working in smaller groups or subsets of larger groups when these groups contained students with similar levels of knowledge. Finally, the relation between question type (algorithmic versus explanation) and engagement depended on the activity topic. In an activity on Solutions and Dilutions, there was a significant relation where algorithmic items had higher occurrences of Interactive engagement. The implications of this work regarding teaching and research are discussed.

Introduction

Active learning (AL) has become an increasingly prevalent teaching pedagogy due to the positive effect on achievement outcomes, particularly for marginalized student populations (Haak *et al.*, 2011; Freeman *et al.*, 2014; Harris *et al.*, 2020). Furthermore, a meta-analysis which looked at multiple research studies that used a variety of different AL techniques in chemistry classrooms showed the effect of AL on achievement outcomes can vary greatly based on the AL technique being implemented (Rahman and Lewis, 2020). For example, one result of this analysis showed that across multiple studies which used Process-Oriented Guided Inquiry Learning (POGIL), the outcomes of POGIL implementation on academic performance ranged from no effect to a medium effect size. One factor that may contribute to this result is cognitive engagement, which has been defined as the effort students put forth towards learning and mastering new material (Fredricks *et al.*, 2004). Therefore, understanding how students cognitively engage while participating in small group activities, and more specifically, identifying what factors may be influencing engagement, could be important in optimizing the positive effect of group work on student performance.

One factor that has been shown to affect student engagement is how long students have been in school. For example, longitudinal studies have investigated student engagement from one to three years and have found fluctuations in the level of engagement students exhibit (Bruce *et al.*, 2010; Kahu *et al.*, 2020). A study among Chinese university students measured student engagement using surveys over a two-and-a-half-year period and found an increase in engagement across this time (Guo *et al.*, 2023). While most longitudinal studies have investigated engagement over multiple years, Kahu et al. analyzed engagement over a single year through narratives provided by interviews and found engagement for first year university students fluctuated throughout the year due to factors such as self-efficacy and sense of belonging (Kahu *et al.*, 2020). Therefore, it can be expected that student's engagement may not even be consistent across a single term as students adapt to their course schedule and become settled into a routine. Additionally, most of these studies have investigated engagement at an institutional level rather than the course level. Students' engagement within a single course may also show variation due to factors related to the specific course content or environment. Therefore, looking at individual students' cognitive engagement across the course of a single term in chemistry classes may offer insights that could provide instructors with actions they could use to improve student engagement.

A second factor that may influence student engagement is group size. Research has shown that group size can have an effect on an individual's learning outcomes, team performance, and learning satisfaction. A review of the effect of group size for elementary, secondary, and post-secondary students showed a negative relation between the number of students in a group and learning outcomes (Wilkinson and Fung, 2002), and that the optimal group size for learning is three to four students (Lou *et al.*, 1996). Work done among secondary school physics students showed that students progressed further in their reasoning when working in groups of four versus pairs (Alexopoulou & Driver, 1996). A study conducted in an undergraduate marketing class demonstrated that group performance increased with number of students in a group up to five students and then decreased (Treen *et al.*, 2016), while a second study investigated the differences between two, three and four person teams on team performance and found that four person teams showed higher performance than two or three person teams (Cossé *et al.*, 1999). Research has also shown that college engineering students who worked in groups of two to four students showed stronger learning satisfaction than those who worked in groups of five to seven students (Chou and Chang, 2018). In summary, previous research indicates that optimal group size may range from three to five students based on its effect on learning outcomes, performance and satisfaction. It may also be dependent on education level (i.e., secondary versus higher education) and subject matter. Although the impact of group size on academic performance and outcomes has been investigated in the literature, we were unable to find similar research on the relation between group size and engagement. However, since research has shown that both engagement and group size can influence learning outcomes, it is possible that group size may also affect student engagement. Therefore, investigating the effect of group size on individuals' cognitive engagement in General Chemistry may provide valuable insight that can be used to optimize student engagement.

The type of question asked in an activity could also contribute to the mode at which students engage. Previous research has shown that achievement outcomes vary depending on whether students were asked to perform a calculation or use a pre-determined set of procedures versus if they were asked questions that were more conceptual in nature (Zoller *et al.*, 2002; Cracolice *et al.*, 2008; Surif *et al.*, 2014). Additional work indicated that questions more focused on calculations promoted lower-order thinking skills whereas questions focused more on concepts and explanations promoted higher-order thinking (Zoller *et al.*, 2002). While question type seems to have an effect on both achievement outcomes and the level of thinking skills students exhibit, it may also be related to the degree to which students engage with the question; therefore, the relation between question type and engagement should be further investigated.

To investigate the effect of the previously mentioned factors on engagement, a way to measure individual students' cognitive engagement is needed. The Interactive-Constructive-Active-Passive (ICAP) framework provides a model which can be used to measure the mode at which students cognitively engage by looking at overt behaviors that students display (Figure 5.1) (Chi *et al.*, 2018). This framework provides an ideal tool to measure cognitive engagement during group work by examining the content of the group conversation as well as non-verbal behaviors (El-Mansy *et al.*, 2022). During group work, in the lowest mode, Passive engagement, students display behaviors which demonstrate that they receive information but do not physically manipulate the information in any way, e.g., nodding in agreement with statements made by members of the group but not writing anything down. In the Active mode, students physically manipulate information but do not generate any new information. For example, students may nod in agreement but also write their answer on their worksheet. For the Constructive mode, students generate new information beyond that which is presented to them. During group work, this may include making statements that demonstrate independent generation of information. At the highest mode, Interactive, students co-generate information through dialogue between students or between students and instructors. This may be posing a question which results in generation of information by another student or answering a question posed by a student.

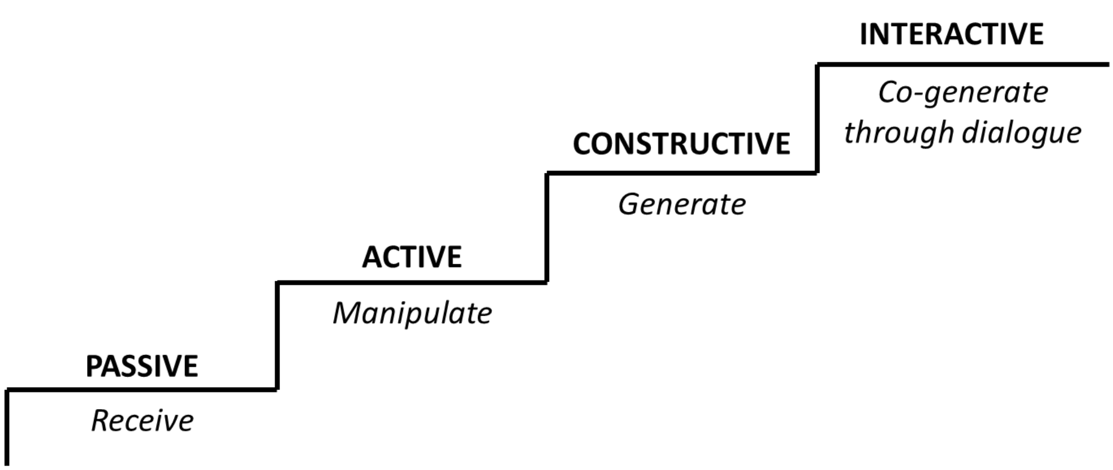

Figure 5.1: ICAP cognitive modes (bold) and characteristic behaviors (italics) (based on Chi et al., 2018)

Research Questions

The purpose of this study is to investigate how individual students within a first term General Chemistry course cognitively engage when working in groups on activity worksheets and to identify factors which may be influencing the level at which they engage. To do so, we used the ICAP framework and deductive coding to answer the following research questions:

1. How does individual students' cognitive engagement vary across activities?
2. What is the effect of group size on individual students' cognitive engagement?
3. What relation is observed between the type of question asked in the activities and students' level of cognitive engagement?

Methods

Setting

Students from two sections of the first term of a General Chemistry course at Portland State University (PSU) in the Pacific Northwest of the United States participated in this study. The course was conducted during the Fall 2022 term (a 10-week quarter), and each section was taught by a different instructor and contained approximately 200 students. The course was taught twice a week for 110 minutes. One day of the week was "lecture" day where the instructor presented the material and engaged students through the use of clicker questions, and the other day was an "activity" day where students generally worked in groups of 3-5 students to complete an activity worksheet. The activity worksheets were developed in-house at PSU and consisted of models which presented conceptual material and/or pertinent equations followed by a mix of calculation-based and conceptual items of increasing difficulty.

Data Collection

The data collected for this analysis was part of a larger research study which was approved by PSU's Institutional Review Board (HRRP# 217370-18). Students were recruited by author S.Y.E. approximately one week prior to each activity being observed. Due to equipment constraints, a maximum of two groups per activity per section were recorded. Groups were capped at five students with the goal of fostering conversation among all group members. Students were selected to maximize racial and gender diversity. These students were then randomly divided into one of the groups for observation. Group sizes varied across the activities and sections based on the number of consenting students who showed up for class on data collection days. Twenty-three students participated across both sections of the course, and six of the twenty-three participated in more than one observed activity. All student names used in this manuscript are pseudonyms.

Three activities were observed during the 10-week term: Solutions and Dilutions in week 3 contained 18 items, Periodic Trends in week 7 contained 37 items, and Molecular Polarity in week 10 contained 24 items. Each group was audio and video recorded for each activity, and the recordings were transcribed verbatim using an automated transcription service. The transcripts were then reviewed and edited by author C.A.S., and pertinent physical actions such as nodding in agreement or pointing to a particular item on the worksheet were added. The completed activity worksheets were collected by author S.Y.E. at the end of the class period. The worksheets were scanned as an additional resource which could be used to aid in the identification of engagement modes. The scanned copies were returned to students the same day as the activity. Additionally, semi-structured interviews were conducted with consenting students approximately one week after the activity day. The purpose of these interviews was 1) to gain insight into the students' perception of the effectiveness of both the activity and the dynamics within their group and 2) as a second data source to triangulate the results obtained from analysis of the recorded observations.

Data Analysis

Individual Coding

Development of the codebook for individual students' cognitive engagement began with a codebook that had been previously developed using ICAP to identify the engagement mode of the group (El-Mansy *et al.*, 2022). In that study, the highest observed engagement mode during group response to an item was identified as the engagement mode of the group for that item. That codebook was applied to group work that was conducted remotely over Zoom and focused primarily on participants' verbal contributions since most of their non-verbal behaviors were not visible in the recording and the overall level of engagement for the group as a whole could usually be determined based on their verbal contributions alone.

During the Winter 2022 term, author S.Y.E. began by applying this prior codebook to each individual student's statements within a group response to a specific item to determine their cognitive engagement. The codebook was first applied to data collected from one group participating in the Molecular Polarity activity during the Fall 2021 term. As coding progressed, S.Y.E. found statements or behaviors that did not align with the code descriptions given in the codebook. To develop the codebook to be more focused on individual students' engagement, during the Spring 2022 term, S.Y.E. met weekly with author A.J.H., an applied linguist, and two undergraduate applied linguistics students, authors A.M. and J.M.F., to analyze conversation excerpts that were difficult to code. Through these meetings, the definitions of each engagement code were expanded and other sources of evidence were looked at, including where students were looking, when students wrote their answers relative to when the group conversation occurred, and their written response on their worksheet. These meetings continued throughout the Spring 2022 term until all ambiguous excerpts were coded to consensus. During the Fall 2022 term, the codebook was further refined by applying it to similar data collected in Spring 2022 from a Physical Chemistry course. This process involved discussing ambiguous excerpts with A.J.H. and an applied linguistics master's student, author S.F., and coding the excerpts to consensus. Additional refinements were made to the codebook, and S.Y.E. used the final codebook (Table 5.1) to code all remaining transcripts from the Fall 2022 General Chemistry classes.

To investigate the effect of when the activity occurred during the term, codes were assigned to each student for each item completed in each activity. For students that participated in more than one activity, the number of codes assigned to a student for each ICAP category were summed, and the distribution of these "summed" ICAP codes was graphed for each activity in which they participated. Trends in these distributions across multiple activities for a single student were then explored.

Table 5.1: Codebook for individual engagement

<table>
<tr><th>UNENGAGED (U)</th></tr>
<tr><td>• Student does not appear to be working on the activity.
    o Makes statements unrelated to activity.
    o Off-task use of their phone.
    o Other behaviors unrelated to working on the activity.</td></tr>
<tr><th>PASSIVE (P)</th></tr>
<tr><td>• Student’s gaze is directed towards other group members or activity worksheet.
• Student may nod in agreement with the conversation regarding the activity but does not orient to the content of the activity in any visible way (e.g., they do not write down any information, do not point to specific parts of the activity).</td></tr>
<tr><th>ACTIVE (A)</th></tr>
<tr><td>• Repeating content from the activity or repeating a statement made by another student in reference to a simple idea (e.g., identifying and writing down something specific from an equation or model).
• Statements or gestures of agreement with an answer provided by another student (e.g., nodding while writing down an answer, giving a “thumbs up”).
• Other evidence of orienting to the content of the activity but without generating new information (e.g., asking what number they are on).
• Students listen to statements/conversation occurring among other students (i.e., orienting to the question) and then write their answer on their worksheet, and/or their written response on the worksheet reflects the content of the conversation.</td></tr>
<tr><th>CONSTRUCTIVE (C)</th></tr>
<tr><td>• Student provides an answer to question, generating new information independent of other members in the group.
    o This may take the form of a statement or a request for confirmation. Other students may agree with the original student’s statement and provide evidence of their own generation of information which does not add any new information to the group.
    o If a single student’s knowledge increases through dialogue, but the group’s does not, this would be CONSTRUCTIVE for that student. (If one student has the answer and “teaches” and others are learning or “catching up”, the original student is CONSTRUCTIVE).
    o If the conversation is about how to solve the problem, and the students write after the discussion, this implies that each student is independently generating information to answer the item because the answer itself has not been co-generated through group conversation.
    o Student may be writing their answer to a specific item prior to conversation about that item among group members and does not alter their written response after the discussion.
    o Student’s written response on their worksheet may show information not present in the group conversation, suggesting independent generation of knowledge.</td></tr>
<tr><th>INTERACTIVE (I)</th></tr>
<tr><td>• Student’s contribution co-generates new information with other students or instructor/learning assistants to answer the item. Neither party shows evidence of generating the answer independently.
    o If the conversation occurs between students, knowledge of more than one group member increases through this conversation.
    o If the conversation occurs between a student and an instructor, the conversation results in co-generation of information for the students engaged in the conversation or for the entire group.
• Student’s statements add to information that has been previously contributed by another student.
    o Student provides new information to answer a question posed by another student.
    o Student poses a question that leads to generation of new information later in the conversation about the question.
    o The generation of new information by the first student prompts a second student to provide additional information.</td></tr>
</table>

To investigate the effect of group size, the number of codes in each ICAP category for each item in an activity for a specific group was determined. For example, for a single item answered by a four-person group, one student was Active, one was Constructive, and two were Interactive. This distribution was determined for every group for every item in every activity. The number of codes for each ICAP category for each group were then summed together. The distribution of these "summed" ICAP codes was plotted across different group sizes, and trends were observed and analyzed.

Question Type Coding

Items in the activities were defined as either "algorithmic" or "explanation". Algorithmic items were defined as those requiring a set procedure or series of steps to determine the answer. Such items may involve a mathematical calculation to determine a numerical solution or require students to recall or apply basic knowledge of a theory. Explanation items were defined as those requiring descriptive explanations, manipulation of algebraic expressions using variables to provide conceptual explanations, or synthesizing multiple pieces of knowledge together to determine an answer.

To investigate the relation between question type and engagement, instances of Constructive and Interactive engagement for each item for each student were tabulated based on question type. While there are four engagement modes, Passive and Active engagement were not investigated in this analysis because students do no generate new information at these lower modes. The Constructive and Interactive modes require students to generate new information, and the difference between these modes is based on whether that generation occurs independently or through dialogue. Therefore, investigating the relation of question type with these modes could provide insight into how and/or why question type promotes dialogue. Each item from each of the three activities was coded as either algorithmic or explanation. The activities were analyzed separately for the relation between question type and engagement mode. This was done to reduce variation caused by the fact that the tasks required by the items for each activity were quite different.

A 2 x 2 contingency table (Figure 5.2) was used to determine if a significant relation exists between the type of question being answered and the Constructive or Interactive engagement mode individual students showed in their response to each item in each activity.

	Algorithmic	**Explanation**
Constructive		
Interactive		

Figure 5.2: Contingency table to compare student engagement with question type

Since a single student is represented multiple times in the dataset, because they answered multiple items, the two categorical variables are not completely independent. Therefore, McNemar’s chi- squared test was used to determine if a statistically significant relation exists.

Data Cleaning

Analysis of the timing and group size factors did not require data cleaning. Because analysis of the question type factor required a statistical test, data cleaning was required. This is because two sources of variation occurred due to the fact that 1) the students across a single activity completed differing numbers of items, and 2) some items had a large number of students who demonstrated Passive or Active engagement or did not answer the item at all. To reduce these sources of variation, the data was cleaned in three steps. First, for each activity, any item that a student did not answer or engaged at the Active or Passive mode was removed for that student. Second, the total number of items that each student answered at the Constructive or Interactive mode was tabulated. If this total was fewer than 50% of the items in the activity, all of that student's responses were removed from the data because by completing such a small part of the activity, these students would not be representative of group work across an entire activity. Third, for each item within an activity, the total number of students who answered the item were tabulated. If this total was fewer than 50% of the students who participated in the activity, the item was removed from the data because such a small sample of student responses to a specific item may not reflect how most students in the group would engage with that type of item. After cleaning, the data consisted of 11 students each in the Solutions and Dilutions and Periodic Trends activities, and 6 students in the Molecular Polarity activity. Six items were removed from the Solutions and Dilutions activity, leaving 12 items for analysis; 3 items were removed from Periodic Trends, leaving 34 items; and 3 items were removed from Molecular Polarity, leaving 21 items.

Trustworthiness

For the individual codes, trustworthiness was established by using investigator triangulation to determine credibility (Lincoln and Guba, 1985; Korstjens and Moser, 2018). This was accomplished through iterative revision of the codebook by authors S.Y.E., A.M., J.M.F., S.F., and A.J.H. until saturation was reached. The remaining data was coded by author S.Y.E. in consultation with author A.J.H. on ambiguous excerpts, and these excerpts were coded to consensus. For question type codes, the codebook was developed by author S.Y.E., and all items on all three activities were coded to consensus with a secondary coder (author A.S.). Data triangulation was also used to assess credibility, with student interviews providing a second data source. The interview responses were used to confirm observed trends of individual engagement across the course of the term.

Results and Discussion

Engagement Across Activities

Six of the twenty-three students who consented to this study participated in more than one activity. Figure 5.3 shows the distribution of each individual's engagement based on the activity they participated in. Tammy, Adriana, Mai, and Melissa participated in both the Solutions and Dilutions (conducted in week 3) and the Periodic Trends (conducted in week 7) activities. All the students except Adriana showed an increase in Interactive engagement; Tammy increased from 50% to almost 90%, Mai increased from 25% to 35%, and Melissa increased from 50% to over 70%. Tammy, Adriana, Melanie, and Molly participated in both the Periodic Trends activity and Molecular Polarity activity which was conducted in week 10; all the students except Adriana showed relative consistency in their Interactive engagement. Tammy's was close to 90% for both activities, Melanie's was approximately 65%, and Molly's was 40%. These results suggest that student engagement within a group may be more likely to change earlier in the term, and their behavior seems to stabilize in the second half of the term. It is possible that students' engagement increases earlier in the term because they are developing patterns in their study behaviors and schedule. Later in the term, students may be more set in their ways and less willing to change their established behaviors.

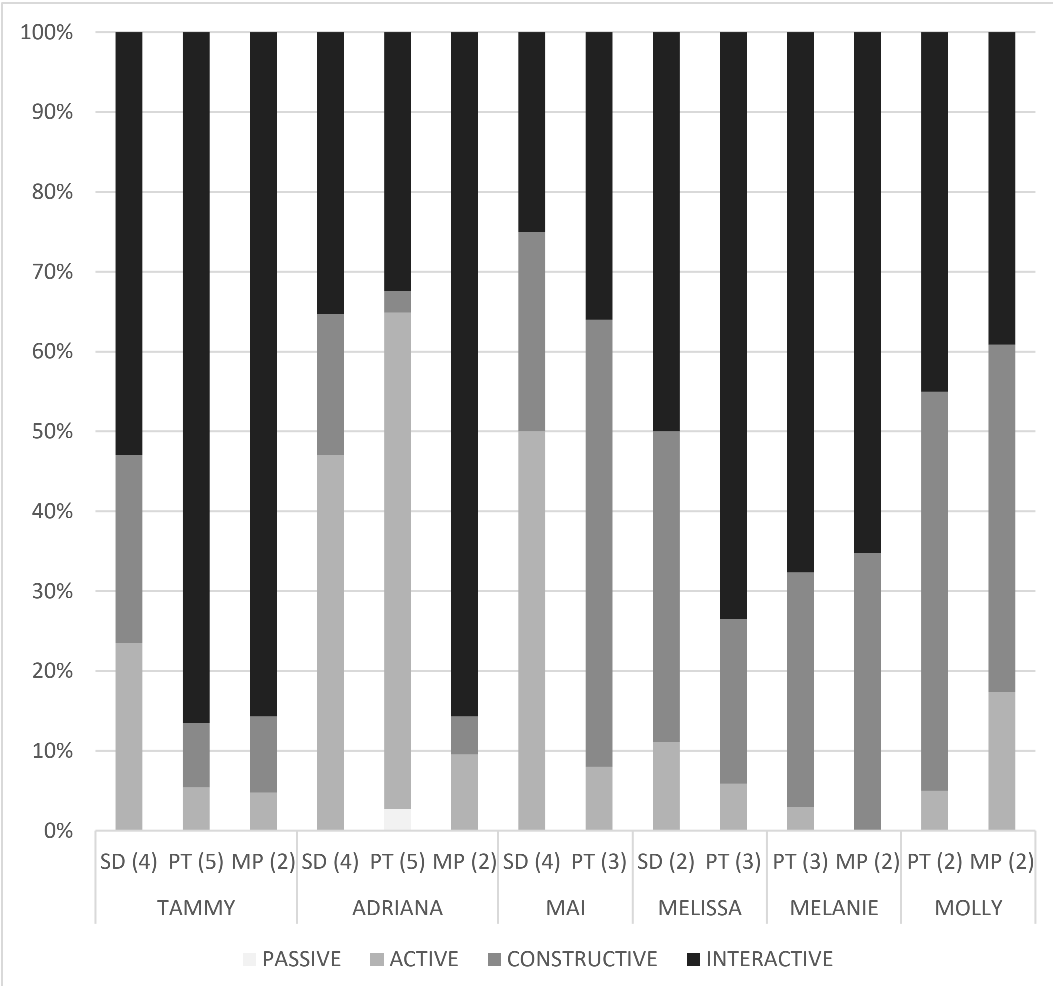

Figure 5.3: Individual student's engagement across activities. SD = Solutions and Dilutions, PT = Periodic Trends, MP = Molecular Polarity. Number in parentheses refers to group size.

However, Adriana did not follow this trend. She participated in all three activities and her Interactive engagement stayed stable around 30% for the first two activities and increased dramatically to approximately 85% for the third activity. For the first two activities, Adriana was in large groups (four people for Solutions and Dilutions and five people for Periodic Trends) and in a small two-person group with Tammy for the

Molecular Polarity activity. During an interview after the Solutions and Dilutions activity, Adriana discussed how working in a group with students whose understanding varied resulted in students working at different speeds. She said (key ideas are in bold):

> "…and I think it matters **what kind of group you're in, what people's levels are**. It is nice to have the variety, the range of like, somebody who doesn't know very much maybe and then somebody who knows more 'cause **if everybody knows a little bit, you can work it together**. But if you are in a group where myself, or the person feels like the others are way ahead, then that gets challenging 'cause you do feel like you're slowing everything down…So having, having a group that's kind of, I don't know if it's better, but **working with people that are a little bit in your range of knowledge or speed of understanding matters** because you don't want to feel like you're the one who's holding the group back from moving onto questions because you still don't understand it or you're just a little slower to understand all the concepts."

Because Adriana felt that the different levels of understanding created pressure on her as a student who did not work as fast (i.e., she did not want to hold up the group from moving forward), this may be what led her to engage more at a lower (e.g., Constructive or Active) mode during the first two activities. Example 1 shows the response of the five-person group consisting of Tammy, Adriana, Anita, Walt, and Kim to Key Question 19 from the Periodic Trends activity (PT-KQ19).

Example 1: Key Question 19 from the Periodic Trends activity (PT-KQ19) and the group response between Anita, Tammy, Walt, Kim, and Adriana

Describe how Boron, Aluminum, and Gallium are similar and different from one another.

2519 WALT: They all have the exact same number of valence electrons.

2520 TAMMY: Yep. Same valence electrons.

2521 ANITA: Also aluminum and gallium are metals. And boron is a metalloid.

2522 TAMMY: It is a metalloid, correct.

2523 ADRIANA: Say it another more time?

2524 ANITA: (speaking to Adriana) So aluminum and gallium are metals. Uh, boron is a metalloid.

Tammy and Walt discussed the fact that the three elements all had the same number of valence electrons (lines 2519 and 2520), and Anita added that gallium and aluminum are metals and boron is a metalloid (line 2521). Adriana began writing her answer after these statements were made. In addition, she asked for Anita to repeat her answer (line 2523), demonstrating that she was working slower than the other group members. Furthermore, her written response contained only the information that was discussed in the group conversation. All these pieces of evidence suggest Adriana demonstrated Active engagement because she was working slower than the rest of her group.

However, in the Molecular Polarity activity, Adriana worked with Tammy in a two-person group, and both students showed approximately 85% Interactive engagement. Example 2 shows their response to Exercise 2a (MP-EX2a). In this excerpt, Tammy and Adriana work together to determine the bond dipoles for the SO_2 molecule.

Example 2: Tammy and Adriana's group response to Exercise 2a from the Molecular Polarity activity (MP-EX2a)

The Lewis structure of SO_2 is provided below (Figure 5.4). Its molecular geometry is bent. (Note: sulfur is an exception to the octet rule.) Draw in the bond dipole moments.

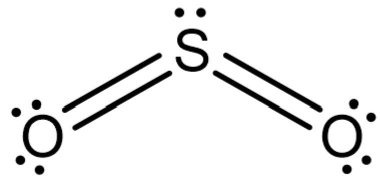

Figure 5.4: Image for Exercise 2a of Molecular Polarity activity

448 TAMMY: So now moving on to 2 with, SO_2, the molecular, it already gives us the molecular geometry, it's bent and sulfur is an exception to the octet rule.

449 ADRIANA: Correct.

450 TAMMY: Draw in the bond dipole moments. So S and O.

451 ADRIANA: So S, I have to look at this and-

452 TAMMY: I have to look up the electronegativity of S.

453 ADRIANA: (points to the periodic table) But I, I think- what's the rule, with the table? Is- it's, it's low to high?

454 TAMMY: I think so-

455 ADRIANA: So-

456 TAMMY: Sulfur is.

457 ADRIANA: Sulfur is less?

458 TAMMY: 2, sulfur's about uh, 2.58 and oxygen I believe...hold on. Oxygen's going to be 3.44.

459 ADRIANA: So it is more.

460 TAMMY: It is way more.

461 ADRIANA: So it should go, oh wait no the other direction.

462 TAMMY: So we want it to be, um, 3.44 minus the 2.58 is 0.86. So the difference is 0.86 and I think they're about equal for each side, right?

463 ADRIANA: Mm-hmm.

464 TAMMY: So one is going 0.86 and it's going away from the central atom and then the other way, 0.86 away from the central atom. Okay, so those are the dipole. So kind of like circle that, that's the dipole moments.

Tammy first recognized that she needed to know the electronegativity of sulfur, and Adriana built upon this idea by mentioning that lower electronegativity values are found in the lower rows on the periodic table (lines 452-453). Adriana also recognized the direction the bond dipoles will point, and Tammy then added on with the numerical electronegativity difference and the fact that the bond dipoles are equal on both sides (lines 461-462). Because Adriana and Tammy seemed to be at the same level of knowledge and were working at the same speed, they both displayed Interactive engagement because they successfully worked together by each contributing pieces of information and combining these pieces to generate the final answer.

Additional insights into how a student engages with both the activity and group members were gained through interview data. For example, during Adriana's interview after the Solutions and Dilutions activity, she was asked about how the activity helped her understanding of the material, and she talked about the importance of understanding why problems were solved in a specific way, not just how:

> "Yeah, because in the moment [during group work], I still felt like I had done the problems, but **I still didn't fully understand where we were grabbing numbers from or why we were putting them in certain orders and what equations we were using**. And so it was one of those where I just copied, I see we're just grabbing numbers, we're placing them in equations, cool, but **I didn't understand the concept behind it and the idea of why we are putting those numbers there and why they should be put there**. So that didn't make sense, I just knew that's how I had to do it. So I was like, cool, I know how I have to do it, now I'll go home and figure out why I have to do it like that."

Tammy was also interviewed after the Solutions and Dilutions activity, and she discussed her positive opinion of group work saying:

> "I've always liked group environment. I like talking things out, I am an auditory learner. I feel that if I am able to talk to someone and hear back, we just converse, and especially if **I'm able to teach it and teach it correctly, then that means I actually understand the concepts**…I don't like just teaching, I like to learn from others as well, like that kind of give and take, that back and forth, so you know, for the majority of the activity, I was in my wheelhouse, I knew what I was doing, so I was kind of leading it, but then as **we were going for more the conceptual things that was where they were coming in, they were teaching me**. I really appreciate it."

Both Tammy and Adriana mentioned the importance of conceptual understanding in their interviews. This attitude is shown in Example 2 by how they worked together to identify the steps and pieces of information needed to determine the bond dipole moments for the SO_2 molecule. The focus on a deeper understanding displayed by both students may have contributed to the development of a strong rapport between them. This may have also resulted in a higher comfort level for Adriana which caused her to more frequently engage at the Interactive mode with Tammy during the Molecular Polarity activity. The high amount of Interactive engagement could also be due to the small group size, which is discussed in the next section.

Group Size

Figure 5.5 shows the distribution of individual engagement codes for all students in a group based on group size, where groups consisted of two to five students. The figure shows variation in engagement levels across group sizes. Given that previous research suggests a positive correlation between academic outcomes and higher modes of engagement (Menekse *et al.*, 2013; Chi and Wylie, 2014), exploring what aspects of group conversations for different group sizes lead to higher engagement could give insights into how to structure effective groups.

Across the five two-person groups, Groups 1-4 showed Interactive engagement of approximately 50% or less. Only Group 5 showed much higher Interactive engagement of approximately 85%. This group consisted of Tammy and Adriana and, as mentioned in the previous section, the high amount of Interactive engagement was likely due to their similar levels of knowledge and goals regarding group work. Since Group 5 was the only group to show such a high level of Interactive engagement, it seems likely that the high Interactive engagement was due to rapport between Tammy and Adriana based on their similar knowledge level and perception of group work, not necessarily the small group size. In the three-person groups, Groups 6 and 7 showed between 60% and 70%

Interactive engagement while Group 8 was much lower (approximately 35%). Groups 7

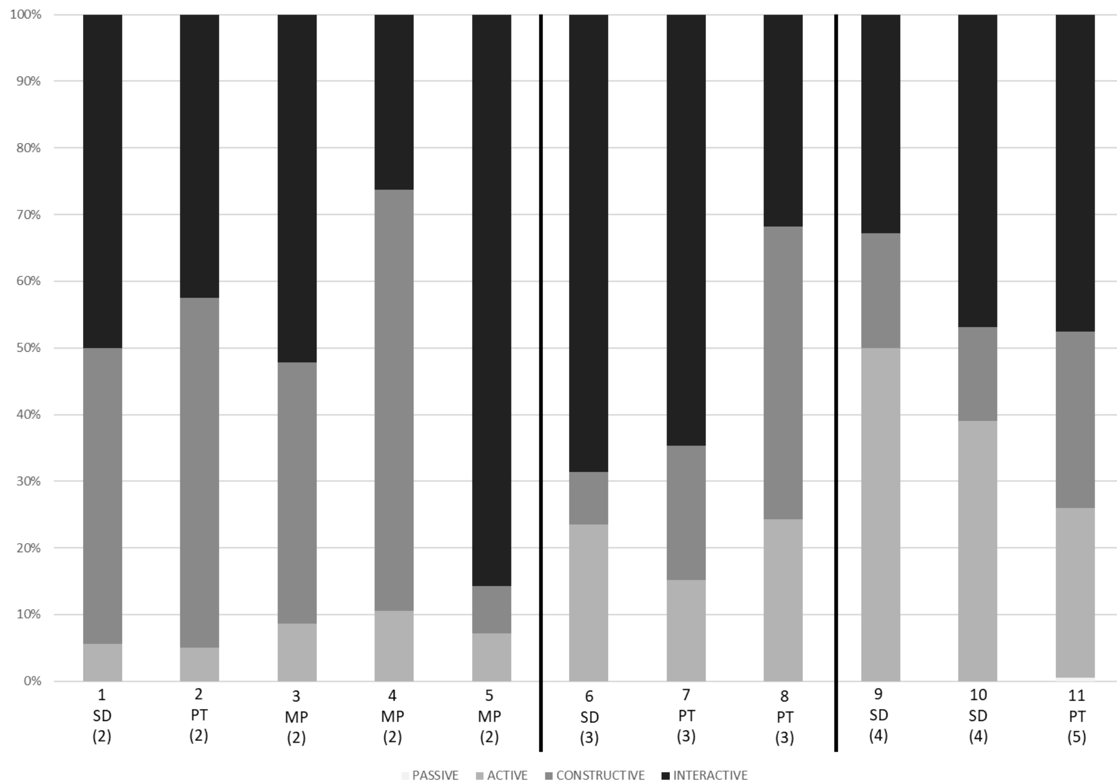

Figure 5.5: Distribution of individual engagement codes based on group size. Activity is identified for each group with SD = Solutions and Dilutions, PT = Periodic Trends, and MP = Molecular Polarity. Number in parentheses refer to number of students in a group.

and 8 both worked on the Periodic Trends activity, and examination of conversation excerpts indicates that in Group 7, the three students seemed to be working at the same pace and knowledge level whereas this was not the case in Group 8. Example 3 shows an excerpt where Group 7, consisting of Mike, Melissa, and Melanie, collaborated to answer Exercise 7 from the Periodic Trends activity (PT-EX7). The students worked together by each contributing information and putting the pieces together to determine the final answer.

Example 3: Group 7's response to Exercise 7 from the Periodic Trends activity (PT-EX7)

What are the characteristics of an electron configuration when IE_1 is high?

1928 MELISSA: Okay. So what are the characteristics of an electron configuration when the, uh, ionization ener-, first ionization energy is high. So it has a free electron, right? It has a-, it has one valence electron.

1929 MELANIE: No, there's, there's none.

1930 MIKE: It's all noble gases.

1931 MELISSA: Oh, when the energy is high. Sorry. Yes.

1932 MELANIE: Yeah.

1933 MELISSA: Yep. Yeah. They're noble gases. So the, the valenc-, the shells are full.

1934 MIKE: Mm-hmm.

1935 MELANIE: Yeah. The shells are full

1936 MELISSA: And the atomic radius is small.

1937 MELANIE: They are happy. And they don't wanna be separated. Snug as a bug in a rug.

In this excerpt, Melissa began by incorrectly stating that an atom with high ionization energy would have a free electron, causing both Mike and Melanie to correct her by offering additional pieces of information; Melanie stated there would be no free electrons and Mike identified these atoms as being the noble gases (lines 1928-1930). Melissa then built on this by recognizing that this meant the valence shell would be full (line 1933). Additionally, the video recording shows that all three students do not write their answers until the conversation is over, indicating that no single student seemed to be working ahead and that the students were all working at the same knowledge level.

In contrast, in Group 8, which consisted of Henry, Rachel, and Mai, the lower amounts of Interactive engagement may be partially due to the disparate levels of knowledge of Henry and Rachel. Example 4 shows part of Group 8's response to Key Question 11, which asks students to describe the trend in ionization energy as one moves down a group of the periodic table. In line 408 below, Henry gives a detailed description of why the ionization energy increases, using the idea of electron shells and referencing the s orbitals. However, the concept of orbitals is not introduced until the next model, suggesting that Henry had prior knowledge of this idea prior to answering this item.

Example 4: Portion of Group 8's response to Key Question 11 from the Periodic Trends activity (PT-KQ11)

Summarize how the first ionization energy changes as you move down a group (column) on the periodic table.

408 HENRY: So I know why it increases or, uh, how do you say the ionization, the energy decreases as you go down a group. As you move farther down, the sub shell count starts increasing. (HENRY uses hands to demonstrate) So like 1s, $1s^2$, and like $2s^2$, like when you reach like, uh, an element like xenon for example, there's a lot more electron configuration that you're gonna have to write down,

(RACHEL and MAI nod heads) which means that the sub shell, there's gonna be a lot more sub shells within that element, which makes it bigger, but it doesn't make it more covalent in terms of a noble gas. But every other element, as it moves down, ionization energy decreases because the radius is increasing.

409 RACHEL: Mm-hmm.

410 HENRY: Because the amount of sub shells are increasing. As you move farther down.

411 RACHEL: Mm-hmm. And that's like pulling apart the electron.

Additionally, Rachel seemed to struggle with understanding the concepts in this activity. For example, Exercise 1 was a multi-part question which asked students to determine between a pair of elements which one had the larger atomic radius. In the first two parts of this item, Rachel made statements such as, “I was confused” or “I don’t understand”. Such statements suggest that Rachel did not have prior knowledge coming into this activity, and this may have contributed to her high amount of Active engagement (33%) compared to Henry (9%). The discrepancy between Rachel’s lack of prior knowledge and Henry’s more advanced level of knowledge may partially explain the lower levels of Interactive engagement demonstrated by this group due to the fact that Rachel demonstrated higher amounts of Active engagement because she waited for someone to “give” her the answer while Henry demonstrated higher amounts of Constructive engagement (42%) because he used his higher level of knowledge to independently answer items or teach his fellow group members concepts as needed. In summary, analysis of conversation excerpts from small and medium groups supports the idea that grouping students with similar amount of prior knowledge may foster an increase in Interactive engagement.

All three of the large groups (Groups 9-11) showed less than 50% Interactive engagement. This may be partially due to the fact that there are cases where not all group members are engaging at the Interactive mode when answering a specific item. For example, Group 10 was a four-person group consisting of Tammy, Amy, Mai, and Zoey. Example 5 shows their response to Key Question 5 from the Solutions and Dilutions activity (SD-KQ5). This excerpt shows that even though Tammy and Amy demonstrate Interactive engagement, Zoey showed Constructive engagement, and Mai engaged at the Active mode.

Example 5: Group 10's response to KQ5 in the Solutions and Dilutions Activity (SD-KQ5)

*The images below (Figure 5.6) represent the same small volume within three different solutions and the spheres represent solute particles (solvent particles are not shown). Which solution has the <u>lowest concentration</u>? Circle your response and **explain** why you chose it.*

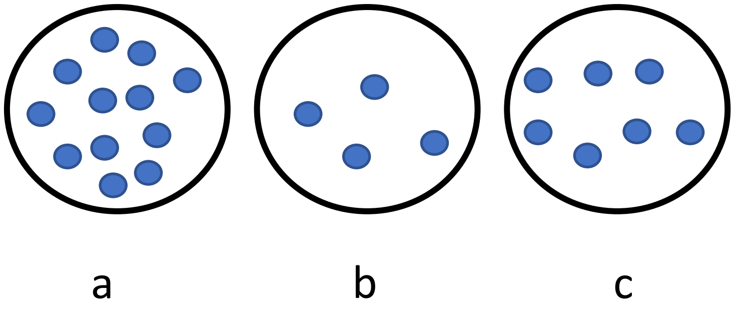

Figure 5.6: Image for Key Question 5 from Solutions and Dilutions activity

396 TAMMY: Okay, cool. Moving on! Number five. Images below represent the same small volume within three different solutions and spheres. And the spheres represent, sorry, solute particles, the solvent particles are not shown. Which solution has the lowest concentration? Circle the response and explain why.

397 AMY: Okay.

398 AMY: Say b, right?

399 TAMMY: I wanna say b.

400 AMY: Yeah.

401 TAMMY: Yeah, 'cause we just established in the last one that concentration means more of whatever the substance is.

402 AMY: Right, yeah. And explain what-. Yeah. There there's fewer...solute particles.

403 TAMMY: Yes. Not more, less. Sorry, less solute.

404 AMY: Mm-hmm.

Both Tammy and Amy were coded as Interactive because they co-generated information to produce the answer. In line 398, Amy said the initial answer, and in lines 401-402, Tammy and Amy co-generated the explanation for that initial answer. Mai was coded as Active because in the video, she looked at Tammy and Amy during their conversation and then looked at Zoey's worksheet prior to writing her answer. Additionally, on her worksheet, she circled option b and wrote, "There are fewer solute particles," nearly replicating Amy's exact wording from line 402. Both the timing of when Mai wrote her response and the content of what she wrote suggests that she simply manipulated information she received from her group members. On the other hand, in the video, Zoey wrote her answer before any conversation occurred. Additionally, on her worksheet, she wrote, "b has less because there are fewer substances inside than the others." This statement is phrased differently than what was said during the conversation, further supporting the interpretation that Zoey independently generated her answer and did not modify it based on Tammy and Amy's conversation; therefore, Zoey was coded as Constructive.

A second factor that may contribute to the lower amount of Interactive engagement is the idea of group splitting. In this group, Zoey and Mai were sitting next to one another and Tammy and Amy were sitting beside each other. The two pairs were across and slightly diagonal from each other. Each "split" group displayed their own engagement pattern, where Zoey and Mai showed higher amounts of Active and Constructive engagement, similar to the other two person groups that were observed (Figure 5.4). Tammy and Amy showed higher amounts of Interactive engagement, which was similar to what was observed between Tammy and Adriana. The larger group size and where the students were seated relative to each other may have been a contributing factor to the high level of interaction between Tammy and Amy and the lower engagement modes from Zoey and Mai. Since the engagement modes shown in Figure 5.5 were determined by summing the engagement modes for all students in the group, this can result in a lower amount of Interactive engagement for the group.

The results of this analysis did not identify an "optimal" group size; instead, analysis of group response excerpts at the different group sizes identified aspects of group dynamics that seemed to facilitate higher modes of engagement. Previous research on group dynamics suggests that one of the primary sources of problems in group environments is the presence of dominant and quiet students in the same group (Hendry *et al.*, 2003; Ahmed, 2014). These studies defined a dominant student as someone who talks a lot and controls the direction of the conversation whereas a quiet student is one who rarely contributes to the conversation. Because it is possible that these characteristics could be related to how knowledgeable (or confident) a student is on a particular topic, our results, which suggest students with differing levels of knowledge in the same group would demonstrate lower levels of engagement, align with these earlier studies.

Question Type

Each activity was analyzed for the relation between the students' engagement mode and the question type. For the Solutions and Dilutions activity, 16 of the 18 items (89%) were coded as algorithmic; for the Periodic Trends activity, 16 of the 37 items (43%) were coded as algorithmic; and for the Molecular Polarity activity, 11 of the 24 items (46%) were coded as algorithmic. The results of McNemar's chi-squared tests indicate there is a significant relation for the Solutions and Dilutions activity but not for the Periodic Trends or Molecular Polarity activities (Table 5.2).

The McNemar's test shows that a significant relation between question type and engagement only exists for the Solutions and Dilutions activity items. This result indicates that students are more likely to engage at the Interactive mode on algorithmic items over conceptual items during this activity. Students engaged at the Interactive mode

Table 5.2: Results of McNemar's test. Numbers in parentheses are the percent of items at the level of engagement for a question type. Bold p-values indicate a significant relation.

		Algorithmic	**Explanation**	
Solutions and Dilutions	**Constructive**	14 (15)	6 (35)	n = 112
	Interactive	81 (85)	11 (65)	χ^2 = 64.655,
	Total	95	17	df = 1 **p = 0.00**
Periodic Trends	**Constructive**	45 (38)	64 (38)	n = 285
	Interactive	73 (62)	103 (62)	χ^2 = 0.59124,
	Total	118	167	df = 1 p = 0.44
Molecular Polarity	**Constructive**	23 (46)	17 (30)	n = 107
	Interactive	27 (54)	40 (70)	χ^2 = 2.2727,
	Total	50	57	df = 1 p = 0.13

81 times on algorithmic items (85%) and 11 times on explanation items (65%). Previous research showed that students use higher order thinking skills on conceptual items and lower order thinking skills on algorithmic items (Zoller *et al.*, 2002); therefore, we initially hypothesized that students may be more likely to engage at a lower mode for algorithmic items. However, our results suggest the opposite trend in this activity. In this study, algorithmic items were broadly defined as including items which required a

mathematical calculation and/or items which required students to use a set of procedural steps to determine an answer. The Solutions and Dilutions activity contained primarily algorithmic items which required students to perform a mathematical calculation whereas the Periodic Trends and Molecular Polarity activities contained procedural-based algorithmic items (e.g., write an electron configuration or draw a Lewis structure), which may account for the differences in the McNemar's test results.

In the Solutions and Dilutions activity, the algorithmic items where conversations had mostly Interactive engagement focused in two areas: 1) students working together to correctly associate numerical values with the correct variables in the dilution equation ($M_C V_C = M_D V_D$), and 2) determining the correct significant figures for their answer. For example, Group 10's (Figure 5.4) conversation related to Exercise 4 from the Solutions and Dilutions activity (SD-EX4) illustrates this pattern (see full excerpt in Appendix B). SD-EX4 asked students to determine the volume of a stock solution needed to produce a known volume of a dilute solution at a known concentration. Tammy and Amy spent a large portion of the conversation attempting to identify what they were solving for and what the V_C and V_D variables referred to. Mai helped alleviate some of their confusion by recognizing that the concentration of the stock solution should be pulled from Model 2. Once the group had identified values for all the variables, the conversation shifted into a discussion of significant figures in which Zoey, Tammy, and Amy worked together to determine that they would need three significant figures. This analysis indicates that multiple facets of calculation-based items, i.e., correct association of numerical values to their appropriate variables and application of significant figures, can promote higher occurrences of Interactive engagement as students work together to complete these tasks.

This group showed lower amounts of Interactive engagement in Key Question 5 from the same activity (Example 5) due to differing levels of engagement of each student and group splitting whereas their response to SD-EX4 showed higher amounts of Interactive engagement and did not show evidence of group splitting. This suggests that question type may contribute to the higher engagement on SD-EX4 versus SD-KQ5; therefore, question type may also influence behaviors that resulted in group splitting observed on SD-KQ5.

Conclusion

While there are many factors that may affect students' cognitive engagement while participating in small group AL activities, this study investigated some factors that are related to the group environment and the activity itself. Specifically, we looked at the effect of timing, group size, and question type. The three factors were explored through the following research questions:

How does students' cognitive engagement vary across activities?

Analysis of six students across three activities throughout the term indicates that in general, students' Interactive engagement increases during the first half of the term but stabilizes during the second half. This data was collected during General Chemistry I, which occurred in fall term and is often a student's first term in college; during this time, students are learning how to navigate the college environment, manage their schedule, and establish study behaviors. Therefore, they may change their approach to various aspects of college, including how they participate in group work, and their engagement may vary as they determine what works best for them. As they become more settled in their college routine, their classroom behaviors, which would include how they participate in group work, may stabilize.

Another possibility is that other factors, such as students' perception of group work and their individual personal goals, may impact their mode of engagement. For example, Tammy had a very positive perception of group work and displayed high levels of Interactive engagement across all activities. In contrast, Adriana's opinion of group work was more reserved, and she mentioned that the success of group work was dependent on the type of group and specifically, people's level of understanding and speed at which they worked. Accordingly, her Interactive engagement remained low in the first two activities where group members worked faster than her but increased in the third activity, where she and Tammy worked at similar speeds with similar goals.

Although students' engagement varied across activities over the course of the term, it is also possible that the topic being presented and the type of questions being asked in the activity may also affect students' engagement, which was explored through the next research question.

What relation is observed between the type of question asked in the activities and students' level of cognitive engagement in General Chemistry?

The results of McNemar's chi-squared test showed a significant relation between question type and engagement mode for the Solutions and Dilutions activity, but not for the Periodic Trends or Molecular Polarity activities. In the Solutions and Dilutions activity, algorithmic items were associated with higher occurrences of Interactive engagement. Algorithmic items in this activity generally asked students to perform a mathematical calculation to determine the answer, and analysis of student conversations indicated that students engaged at the Interactive mode to correctly associate numerical values with the appropriate variables and to correctly apply significant figures. Although this result was significant, 89% of the items on the Solutions and Dilutions activity were algorithmic, resulting in a skewed dataset. In comparison, the Periodic Trends and Molecular Polarity activities had a more balanced distribution of algorithmic and explanation items (43% and 46% algorithmic items, respectively). Since there were very few explanation items in the Solutions and Dilutions activity, this analysis should be repeated with a more balanced spread of algorithmic and explanation items to determine if a significant relation would be obtained again.

In addition to having a better balance between the different question types, the algorithmic items in the Periodic Trends and Molecular Polarity activities did not involve calculations but instead asked students to apply a set of procedural steps to complete a task. Although the raw data in Table 2 does show higher occurrences of Interactive engagement on algorithmic items for these activities, the relation is not statistically significant.

Since timing and question type both affect engagement, there may be conflation between these factors. For example, the Periodic Trends and Molecular Polarity activities had similar proportions of explanation items and they both occurred during the second half of the term. For students who showed an increase in Interactive engagement from the Solutions and Dilutions activity to either the Periodic Trends or Molecular Polarity activity, this may be due to a combination of the effects of timing and question type.

What is the effect of group size on individual students' cognitive engagement?

The results of this analysis do not definitively suggest an “optimal” group size; however, the analysis did highlight the fact that higher amounts of Interactive engagement occurred in groups that contained two or three students when the students in these groups had similar levels of prior knowledge. In larger groups of four or five students, lower amounts of Interactive engagement were observed. This is because only a portion of the group typically demonstrates Interactive engagement, while the remaining students show lower modes of engagement. In these larger groups, students may be more likely to split into sub-groups where each sub-group would have a different group dynamic. Depending on multiple factors affecting group dynamics, including perceptions of group work and students’ level of prior knowledge, these smaller groups could resemble the previously observed engagement distributions for smaller groups.

Further analysis into the effect of group size on engagement found that behaviors such as group splitting were not consistent within a single group on an activity. This result suggests that there may be interplay between the various factors investigated in this study.

Limitations

This study investigated the effect of timing, group size, and question type; however, individual student characteristics, such as gender identity, students’ aspirations, and academic capability (Fullarton, 2002; Lee *et al.*, 2022), may also influence a student’s engagement and may contribute to the observed results. As this is a qualitative study with a small sample size from a single term of a General Chemistry I course, these results may not be generalizable to other courses or activities. Additionally, the ICAP framework assumes that the overt behaviors students display are reflective of their internal cognitive engagement; however, this may not always be the case. For example, students may independently generate information (Constructive engagement) while their conversation may show only Active modes. In future studies, additional reflective interviews with students while they are reviewing the group interaction video, i.e., stimulated recall, may be able to address this (Dempsey, 2010). In addition, the observed groups in this study did not remain the same across multiple activities. Therefore, for each activity, students were working with new peers for the first time and had to learn how to communicate and work together. Since students may interact with one another differently with a different set of group members, the engagement of individual students may have been affected. Finally, this work looked at unstructured groups, and the results may not be applicable to highly structured groups, such as those used in POGIL. While POGIL groups are larger, generally containing 4-6 students, each student is assigned a specific role (e.g., manager, recorder, reflector) (Farrell *et al.*, 1999). The duties of each assigned role may affect that students' engagement; for example, the recorder may show lower modes of engagement using ICAP as their primary role is to record the group's thoughts and answers, and as a result, may be less likely to verbally contribute information to the conversation.

Implications for Instructors

The results of the analysis of students' engagement across multiple activities suggest that there may be opportunities for instructors to influence students early in the term. The stabilization of engagement in the second half of the term (during the Periodic Trends and Molecular Polarity activities) suggests that students may have established their academic habits and may be less willing to change. Therefore, we would encourage instructors to continually emphasize the benefits of group work and specifically the type of conversations in which students should be engaging. While it is possible that changes in engagement across the term may not be solely due to timing, there may be conflation with the type of questions being asked. Instructors could address this by giving examples of what productive conversations would look like for different question types. For example, instructors may want to encourage students to talk through the specific steps of an algorithmic item requiring a mathematical calculation or clearly discuss their thought processes behind their answer when asked to make a prediction on a conceptual item.

The group size analysis suggests that students should work in smaller groups and that students with similar knowledge levels should be grouped together to enhance productive conversation and Interactive engagement. While it may be difficult to determine which students have similar knowledge levels and group them accordingly, we encourage instructors to have students form smaller groups whenever possible and continually emphasize the importance of *all* students participating in the group conversation, regardless of size. We would also suggest that instructors continually discuss the idea that group work is intended to improve the understanding and knowledge of all students and that each student may be able to bring different insights or perspectives to the activity. The instructors can highlight that this will occur through conversations with fellow group members.

Implications for Research

This study analyzed the engagement of individual students in a group environment and found that factors such as timing, group size, and question type may affect individual students' engagement. Although previous research found a correlation between higher modes of engagement and improved achievement outcomes (Menekse *et al.*, 2013; Chi and Wylie, 2014; Wiggins *et al.*, 2017), further research is needed to explore the relation between these factors which influence engagement and learning outcomes. In addition, research into individual students' engagement when group composition remains constant may provide additional insight into the effect of other factors on engagement, such students' sense of belonging, active learning environment, and instructor support (Gasiewski *et al.*, 2012; Wilson *et al.*, 2015; Craft and Capraro, 2017; Struyf *et al.*, 2019; De Loof *et al.*, 2021). Finally, the analysis of Tammy's and Adriana's engagement suggests that students' perceptions of group work and individual student goals regarding the activities may influence their engagement as well and should be explored.

Conflicts

There are no conflicts of interest to declare.

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Chapter 6: Improving Physical Chemistry Activities: Using Scaffolding to Reduce Cognitive Overload in Hydrogen Atom and Harmonic Oscillator Worksheets

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El-Mansy collected and analyzed data, designed activities, wrote manuscript; Barbera revised manuscript; Hartig revised manuscript; Shusterman designed activities, wrote and revised manuscript.

Abstract

Two activity worksheets for the quantum mechanics section of a Physical Chemistry class are presented in this article. These worksheets modified original instructor-developed worksheets to reduce cognitive overload by incorporating scaffolded items to help students perform pertinent mathematical calculations and improve conceptual understanding. Observation of student groups, student interviews, and instructor insights into the effectiveness of the redesigned worksheets suggest that the worksheets were successful in breaking down complex ideas and in helping students better grasp the concepts being presented.

Graphical Abstract

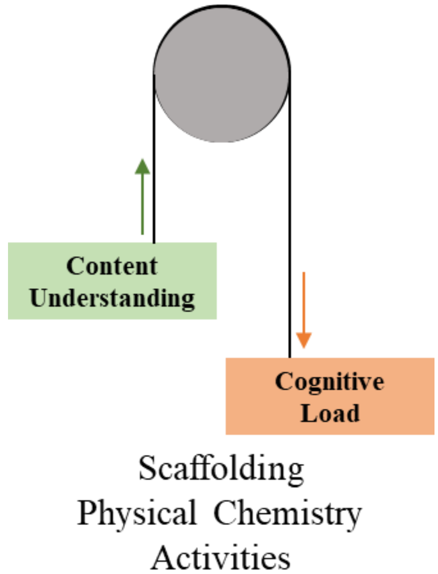


Figure 6.1: Graphical abstract representing how Physical Chemistry activities are scaffolded

Keywords

Physical Chemistry, Quantum Mechanics, Collaborative / Cooperative Learning, Student-Centered Learning

Introduction

Within upper-division chemistry courses, such as the quantum mechanics term of Physical Chemistry, students often face challenges such as the abstract and complex nature of the topic as well as the complex mathematical knowledge required to complete calculations (Dangur *et al.*, 2014; Greca and Freire, 2014; Tsaparlis and Finlayson, 2014). These challenges may be a result of cognitive overload. Cognitive load theory (CLT) suggests that an individual's working memory capacity is limited; therefore, when learning new material, if the learning tasks are too complex and require capacity greater than that available in the working memory, learning is hampered (Van Merriënboer and Sweller, 2005; de Jong, 2010). CLT aims to improve student learning by designing instructional systems to reduce cognitive overload. Cognitive load theory identifies three types of load: 1) intrinsic load which is the difficulty or complexity of the subject materials, i.e., the number of different elements that interact for students to learn a concept; 2) extraneous load which is imposed by factors in the instructional design which do not contribute to learning; and 3) germane load which is created by the learning processes students use, e.g., interpreting, classifying, or organizing (Paas *et al.*, 2003; de Jong, 2010). The majority of previous work done in this area has focused on designing learning tasks to reduce extraneous load, with a small number of studies looking at reducing intrinsic load (Paas *et al.*, 2003; Van Merriënboer *et al.*, 2003, 2006; Ayres, 2006).

Research also suggests that active learning and specifically, active learning which incorporates small group work, leads to improved academic performance in science, technology, education, and mathematics (STEM) courses (Freeman *et al.*, 2014; Rahman and Lewis, 2020). One facet of small group work that can be optimized to address the challenges students face in a specific course may be the activity or learning tasks themselves. When students are learning quantum mechanics, they face intrinsic load imposed by the complex nature of the subject. Students may also deal with extraneous load caused by the manner in which the questions are being asked. The cognitive overload caused by these sources can be mitigated by designing activity worksheets in a way to reduce this load and improve student understanding. Therefore, insights into where student struggles occur may provide a driver towards designing the materials used during group work (e.g., learning activity worksheets) to optimize student learning.

One possible way to reduce cognitive overload in activity worksheets is the inclusion of scaffolded questions. "Scaffolding" refers to simplifying a task by breaking it down into its constituent parts (Wood *et al.*, 1976). Research has shown that the implementation of scaffolding by creating a sequence of tasks that move from simple to complex reduces intrinsic load by reducing the high element interactivity found in complex questions (Paas *et al.*, 2003; Van Merriënboer *et al.*, 2003, 2006; Van Merriënboer and Sweller, 2005; Ayres, 2006). Additionally, studies in STEM education have suggested a positive relation between the implementation of scaffolding and learning outcomes (Belland *et al.*, 2017). Research also suggests that learning is a constructive process where new knowledge builds upon existing knowledge, and activating the existing knowledge may provide a framework for learning (Gijselaers, 1996). These ideas can contribute to the design of learning activities, where in addition to reducing cognitive load, the inclusion of scaffolded questions may allow students to build upon existing knowledge to create new knowledge.

While workbooks with active learning activities such as Process Oriented Guided Inquiry Learning (POGIL) (Moog and Spencer, 2008) exist, these types of published materials can add costs to a class. Additionally, the materials within published workbooks may not be customizable to meet an instructor's needs in best supporting their students. Here, we present two activities, a Hydrogen Atom and Harmonic Oscillator worksheet, which were developed during the quantum mechanics term of a Physical Chemistry class. These learning activity worksheets were developed based on the principles of scaffolding with the purpose of guiding students to build on their existing knowledge in order to better connect their mathematical reasoning to conceptual knowledge from the course.

Activity Design Goals

The primary goal of designing these activity worksheets is to reduce cognitive overload when learning concepts in quantum mechanics. Previous research suggests that one source of overload is the high level of math proficiency required in Physical Chemistry (Nicoll and Francisco, 2001). While math knowledge may contribute to overload in multiple ways, this paper addresses two of them. First, complexity – when the math needed to solve problems contains multiple ideas, students' attention may become focused on the procedural aspect of solving the math instead of learning the chemistry concept. Therefore, the math complexity is a source of intrinsic load due to high element interactivity that occurs from combining multiple math ideas to solve a problem. Second, information overload – the use of multiple terms and units for the same concepts can cause students to process and digest too much information in their working memory. By using multiple terms, students are using their working memory on ideas that do not contribute to learning, i.e., extraneous load. The Hydrogen Atom and Harmonic Oscillator activity worksheets were designed to reduce intrinsic and extraneous load by using scaffolding to break down complex ideas into smaller, manageable pieces and to minimize information overload.

Development of Scaffolded Activities

The quantum mechanics section of Physical Chemistry was taught during the spring term, three days a week, for 65 minutes. Most class sessions began with a mini-lecture followed by a group work session where groups of 3-5 students collaborated to answer questions on an activity worksheet. Data collected for this work was part of a larger research study, and Institutional Review Board (IRB) approval was received from Portland State University (HRRP# 2007004-18). Groups were audio and video recorded during the Spring 2021 term when the original instructor-designed worksheets on the Hydrogen Atom and Harmonic Oscillator were used. Based on these observations, author S.Y.E. and the course instructor (author G.S.) identified areas of struggle or confusion and redesigned the worksheets using the principles of scaffolding to reduce student cognitive overload and improve conceptual understanding. The redesigned worksheets were then administered during the Spring 2022 term, and group work was again audio and video recorded to evaluate the worksheets' effectiveness. Student interviews were also conducted to evaluate their perception of the redesigned worksheets. The complete

Hydrogen Atom and Harmonic Oscillator worksheets are available in Appendix C. Figures 6.1-6.3 show example items from both worksheets.

Each worksheet listed the learning goals for the activity, which included comprehension of simple concepts that then built to larger, complex ideas (see Supporting Information). For the Hydrogen Atom worksheet, one learning goal was for students to understand the relation between Cartesian and spherical polar coordinates and specifically, to identify the mathematical form of dτ and the integration limits in both coordinate systems. To accomplish this goal, an item from the original Hydrogen Atom worksheet asking students to evaluate a triple integral was evaluated (Figure 6.1a). This item has high element interactivity, i.e., intrinsic load, as students needed to apply multiple new concepts simultaneously to determine the correct answer. Specifically, students had to correctly identify the coordinate system being used, understand what variables are included in the dV term, know the limits of integration over all space for the correct coordinate system, and know how to correctly evaluate a triple integral. Observations from the Spring 2021 term indicated that students struggled to successfully combine these skills to answer the item.

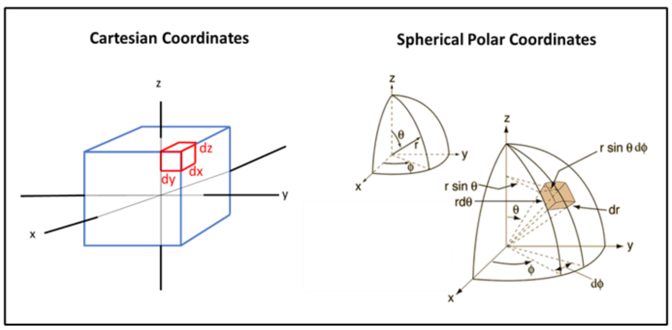
To reduce intrinsic load, this item was redesigned by first presenting a model where a familiar concept (i.e., Cartesian coordinate system) was compared to the new concept (i.e., spherical polar coordinate system) (Figure 6.1b). Students also were confused by the use of the dV term in the three-dimensional integral in the original item. To alleviate this confusion, the more generic $d\tau$ term was used in the redesigned item. Scaffolded items were added to address each concept individually. Students were first asked to identify specific elements for the familiar system (items 1a and 1b) and then asked for the same information for the new system (items 1c and 1d). By breaking down the item in this manner, the high element interactivity of the original item was eliminated. As a last step, they were asked to evaluate the triple integral (item 2). In part 2a, students used the knowledge gained from item 1 to recognize which coordinate system they would be working in and then they combined all the pieces together to solve the integral in part 2b.

a

Evaluate the integral below over all space.

$$\iiint e^{-2r} \cos^2\theta \, dV$$

b



1. a) Write down the volume element $d\tau$ for the Cartesian coordinate system.

   b) What are the limits of integration over all space for the Cartesian coordinate system?

   c) Write down the volume element $d\tau$ for the spherical polar coordinate system.

   d) What are the limits of integration over all space for the spherical polar coordinate system?

2. a) Look at the integral below. Does this integral use Cartesian or spherical polar coordinates?

$$\iiint e^{-2r} \cos^2\theta \, d\tau$$

   b) Evaluate the above integral over all space.

Figure 6.2: a) Item from original instructor-designed Hydrogen Atom worksheet b) Model and scaffolded items in redesigned Hydrogen Atom worksheet

In the Harmonic Oscillator worksheet, one of the learning goals was for students to recognize that wavelength, frequency, and wavenumber are all used as different representations of energy. Figure 6.2a shows an item from the original Harmonic Oscillator worksheet where the students were asked to first determine the zero-point energy of a carbon monoxide (CO) molecule and then calculate the infrared (IR) frequency. To calculate the energy (part a), students needed to use an equation that includes variables for force and mass, and they needed to understand how the units for force and mass relate to the units for energy. To determine the IR frequency (part b), students had to understand the relation between frequency, wavelength, and wavenumber, and the appropriate units for each. Observations from the Spring 2021 term suggested that students struggled with extraneous load as they processed too much information while attempting to apply the correct relations between variables and units. To address this, Figure 6.2b shows new scaffolded items that were added to the redesigned worksheet with the intent of creating a sequence of simple to complex items first activating students' prior knowledge about the relation between frequency, wavelength, and wavenumber and their units, and a new item deconstructing Newtons into its component SI units was added (items 1-3). In addition, a new conceptual item was presented to reinforce student understanding relating bond strength, wavenumbers, and force constants (item 4).

Students also struggled to answer item b (Figure 6.2a). They needed to understand multiple concepts, i.e., what the zero-point energy represents and that the IR frequency is related to the concept of an energy *change* from a ground state to a higher energy state.

a

a) Determine the value of the zero point energy (n=0) of CO in J/molecule and kJ/mol.

b) Determine the IR frequency (cm^{-1}).

b

1.

a) What is the mathematical relation between wavelength (λ) and frequency (υ)?

b) What are the units of each variable?

2.

a) Describe in your own words how wavenumber relates to wavelength and frequency and provide an equation showing the relation. (Note that although chemists refer to IR “frequencies”, these numbers are actually reported in units of *wavenumbers*).

b) What are the units for wavenumber ($\tilde{\upsilon}$)?

3. The Newton (N) is a derived unit composed of SI base units. Break down the Newton into its component units.

4. A C-N single bond, C=N double bond, and C≡N triple bond will have IR frequencies at roughly 1100 cm^{-1}, 1660 cm^{-1}, and 2220 cm^{-1}, respectively. Use your knowledge of the relation between frequency and force constant to match each force constant to its corresponding C-N bond. NO CALCULATION NECESSARY!

1.	$C \equiv N$	*A.*	$1047.6\ N/m$
2.	$C = N$	*B.*	$1873.7\ N/m$
3.	$C - N$	*C.*	$460.0\ N/m$

Figure 6.3: a) Item from original instructor-designed Harmonic Oscillator worksheet b) Scaffolded items and new conceptual item in redesigned Harmonic Oscillator worksheet

To address the high intrinsic load created by this item, a new item was added to help students recognize that the IR frequency (i.e., wavenumber) refers to an energy *transition* (Figure 6.3, part b) and part c was reworded to connect the ideas of wavenumber and energy.

The force constant for a CO molecule is 1860 N/m.

a) Calculate the zero-point energy for the CO molecule (in J/molecule). (Molar mass of carbon = 12.01 g/mol; molar mass of oxygen = 16.00 g/mol). REMEMBER UNITS!

b) How much energy (in J) is needed for a single CO molecule to move from the ground vibrational state to the first excited vibrational state?

c) What wavenumber does this correspond to? (This would be the peak position on an IR spectrum).

Figure 6.4: Redesigned item in Harmonic Oscillator worksheet with additional scaffolding (part b)

Assessment of Scaffolded Activities

The effectiveness of the redesigned worksheets was evaluated by observing group work on these worksheets during the Spring 2022 term. Figure 6.4 shows one group's response to the scaffolded items from the Hydrogen Atom worksheet (Figure 6.1b). In this response, Zane, David, and Connor were able to correctly identify key information (the volume element and integral limits) for the familiar and new concepts (Cartesian and spherical polar coordinate systems) to answer item 1a-d (lines 8-15). They also recognized the fact that the integral is in spherical polar coordinates (item 2a). Furthermore, answering these scaffolded items helped the group correctly evaluate the triple integral in item 2b (lines 18-27).

Figure 6.5 shows a group response to the redesigned item in the Harmonic Oscillator worksheet (Figure 6.3). The scaffolded items a and b seemed to help the students conceptually understand that two energy calculations were needed (lines 247 and251). Furthermore, breaking the item down into these pieces allowed David to understand that an energy transition was occurring and that was the energy needed in the

Response to item 1a
8 CONNOR: So the volume element is just dx dy dz for the Cartesian coordinate system?

Response to item 1b
9 CONNOR: I'd say the limits for that would be infinity in all directions.

Response to item 1c
10 DAVID: For c, just write what she wrote? What she wrote.
11 ZANE: $r^2 sin$ ...

Response to item 1d
12 ZANE: x is zero to infinity, or r...
13 DAVID: What's the other one called?
14 ZANE: ϕ, zero to 2π.
15 DAVID: Zero, right.

Response to item 2a
16 CONNOR: Spherical polar.
17 ZANE: Okay. <laugh> So...

Response to item 2b
18 CONNOR: It's basically taking the integral three times...I forget the rules for doing...
19 DAVID: I think we can integrate whichever one we want first. The bottom one would be for r since we have the r^2 and then e^{-2r}, once you put in the $d\tau$ into it. And then the middle one would be integrating for θ. Cause it's just the $cos^2\theta$.
20 CONNOR: Okay. I see. Um, so each integral is with respect to one of the three variables? Okay. I was trying to look at it as all, like one thing, I think that's why I was getting confused.
21 DAVID: Yeah. So like, since you have the $dr\ d\theta\ d\phi$, and we have like all of the space for it, we just integrate over each one of these variables individually.
22 CONNOR: Yeah. So you'd pull everything out basically.
23 DAVID: Yeah. Yeah. So it's like integrate over r, you get like that, and then you take that entire thing plus what you didn't use to integrate over the next term. And then you do that again.
24 CONNOR: Yeah. Could you also split it up even like...
25 DAVID: If we don't have the dr or $d\theta$.
26 CONNOR: Okay. But this encompasses all of that, right?
27 DAVID: Yeah.

Figure 6.5: Group response to scaffolded items (Figure 6.1b) in the redesigned Hydrogen Atom worksheet

calculation (line 258). In addition, David's response highlighting the relation between wavelength and wavenumber may be a result of the clarifying language used in item c. The group response to this item suggested that the addition of items b and c helped students to connect the idea of an energy transition with the appropriate mathematical calculation.

Further support for the success of these redesigned worksheets was gathered through interview data. Zane was interviewed after participating in the redesigned Hydrogen Atom worksheet. When asked about what the focus of the group conversations

Response to question a
247 CONNOR: The zero point energy is just, uh, $n = 0$.
248 DAVID: Yeah.
249 CONNOR: Okay. What was your answer?
250 DAVID: Uh, 2.13×10^{-20}.

Response to question b
251 ZANE: So this would be...the next one we're just doing $n = 1$?
252 CONNOR: I think so. Yeah.
253 CONNOR: What did you get?
254 DAVID: Um, 4.26×10^{-20}.

Response to question c
255 CONNOR: Yes. And then you just did the, uh, frequency equals c times the wavelength uh wavenumber, sorry?
256 DAVID: Let me give you the...
257 CONNOR: Sorry?
258 DAVID: That'll give you the, uh, since the frequency is the same, um, for...If we're using the same frequency, um, I think, won't that be..? Uh, it won't like tell us that like transition. I mean, I did, uh, I did $\Delta E = hc/\lambda$. So $\lambda = hc/\Delta E$, got a value for λ and then took the reciprocal of that and got 2144.5?
259 CONNOR: Yes.
260 DAVID: Uh, wavenumbers.
261 CONNOR: That makes sense.

Figure 6.6: Group response to redesigned item (Figure 3) in Harmonic Oscillator worksheet

was, he mentioned the benefit of the scaffolded items by saying, "…and this [activity] broke it down, you know, instead of just reading a bunch of information, trying to piece it together, I think the worksheet did a really good job at, you know, the first section, just kind of roots the problem and then building your way up to harder and harder problems." Zane was then asked to elaborate on how the scaffolded items were helpful, and he said the items "…[helped] to separate the difference between Cartesian and spherical polar coordinates and kinda show how they are similar, but how using spherical coordinates definitely are much easier, when it comes to this class at least." These quotes suggest that the use of scaffolding in redesigning the worksheets was effective in reducing some of the confusion created by the high level of intrinsic load previously observed in this activity.

Connor was interviewed after participating in the Harmonic Oscillator worksheet. When he was asked about which items were helpful for understanding the material, he identified the item in Figure 6.3 as being particularly helpful. He said, "I felt like [it] kind of took us through everything, 'cause we were looking at the energy difference. Um, and then we're also correlating that with the wavenumber, which is kind of everything all encompassing." Connor was then asked what he thought the learning goal behind this item was and replied, "…we have to calculate that transition and then find what wavenumber it corresponds to. So I feel like it was just kind of like the, the last thing in it, you know, just like that, that was the, the ultimate goal of our understanding of this was to be able to make that connection and to be able to do the calculation as well." These quotes again reinforce how the inclusion of these additional items in the activity encouraged students to put the individual pieces together to connect conceptual knowledge and mathematical calculations.

Additionally, the instructor of the course (author G.S.) provided her insights into the effectiveness of the worksheets. In the Hydrogen Atom worksheet, G.S. spoke about how the inclusion of scaffolded items in the redesigned worksheets resulted in students applying their efforts in appropriate places rather than getting unnecessarily sidetracked. For example, instead of spending a lot of time attempting to define the differential element $d\tau$, the model and scaffolded items (Figure 6.1) reduced cognitive overload by helping students quickly set up the problem with the correct differential element and integration limits. The students were then able to spend more time and cognitive load on actually evaluating the integral. Similarly, in the Harmonic Oscillator worksheet, the items focused on units (Figure 6.2b, items 1-3) clarified the relations, and the students did not spend time and extraneous load being "stuck" as they had with the original worksheet. Furthermore, G.S. spoke of the inclusion of the new conceptual question

(Figure 6.2, item 4) and its effectiveness in helping students make connections between concepts being taught in the course (i.e., the relation between IR frequency and bond order) and experiences the students have in the lab (i.e., collecting IR spectra and using peak positions to identify functional groups). G.S. also said that she believed that the idea of the interaction between light and matter resulting in an energy *transition* is the most important concept of the term and that the improved scaffolding of the item in Figure 6.5 helped cement this idea in students' thinking.

Conclusion

The redesigned Hydrogen Atom and Harmonic Oscillator worksheets presented here appear to reduce student confusion and improve student understanding by minimizing overload caused by intrinsic and extraneous load. These results came from a small qualitative study that was conducted in one course. As instructors facilitate the use of these worksheets in their own classes, they can pay attention to the direction of conversation among students to determine how successful the worksheets are within their course. Furthermore, instructors can use this insight to adapt the worksheets to their own students' needs.

In general, this work has demonstrated that through the use of scaffolded items to break down large, complex concepts into smaller, more manageable pieces, students struggled less. The course instructor observed that students progressed further through the worksheet than they had when less scaffolding was present. The addition of items to both focus students on mastering conceptual learning and help students connect specific concepts to mathematical calculations elicited a positive reaction. We provide these worksheets as an editable resource for Physical Chemistry instructors to use in their own classrooms to help students break down and simplify some of the complex concepts which are taught in quantum mechanics.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available in Appendix C and includes the Hydrogen Atom and Harmonic Oscillator activities and corresponding keys.

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Chapter 7: Conclusions and Implications

Conclusions

This dissertation research conducted a qualitative investigation into how students cognitively engage when participating in group work in chemistry courses. Although small group active learning has a positive effect on achievement outcomes, the magnitude of this effect can vary widely (Rahman and Lewis, 2020). Understanding the role of cognitive engagement during group work and what factors affect engagement can help explain and minimize some of the observed variation. Therefore, this dissertation sought to investigate the role of cognitive engagement in group work and the various factors that may affect engagement through the four research questions proposed in Chapter 1.

One key component of student learning during group work is the discourse that occurs between students. Therefore, to understand the role of cognitive engagement during group work, student discourse was analyzed using the Interactive-Constructive-Active-Passive (ICAP) framework which identifies the mode of cognitive engagement based on overt behaviors students display. ICAP was used to evaluate cognitive engagement at two grain sizes. In Chapter 4, the expected engagement of student groups was compared with the observed engagement of the groups in an Honors General Chemistry class, and instances of mismatch were analyzed for common themes (RQ 1). Chapter 5 focused on the engagement of each individual student within a group in a General Chemistry class and identified factors that influenced students' engagement (RQ 2). Additionally, other factors such as the type of question students were asked in activity worksheets, i.e., algorithmic items, which were more calculation-based, versus explanation items, which were more conceptual in nature, were investigated (RQ 3). Finally, in Chapter 6, the structure of the activities students worked on in groups during a Physical Chemistry course was analyzed and modified to potentially improve student engagement and learning.

RQ 1. a) How do student groups' expected and observed cognitive engagement align while participating in small-group active learning activities in chemistry courses?

b) What themes may contribute to any observed misalignment?

Expected engagement modes were identified for each item in the activities in an Honors General Chemistry class based on what the item asked students to accomplish. Results showed that engagement modes were not consistent across the entire activity as previous studies indicated (Menekse *et al.*, 2013; Wiggins *et al.*, 2017). The observed engagement modes of the groups were also determined for each item based on the content of the group conversation. Like the expected engagement modes, these results also indicated that the engagement of the groups was not consistent across the course of an activity. For the majority of items, groups demonstrated Interactive engagement. However, the engagement modes were not consistent across all groups for the same items in an activity.

Cases of mismatch were identified when the expected and observed engagement modes for specific items did not align. Across the observed activities, the expected engagement modes were mostly Constructive or Interactive engagement with some instances of Active engagement. When compared to the observed engagement modes, the analysis found that mismatch occurred when groups were expected to engage at the Active mode because the answer to a specific question was provided in the models in the worksheet, but the groups actually engaged at the higher Constructive or Interactive mode. Thematic analysis was applied to the group conversations for these items, and three themes were identified as sources of the mismatch. The first theme related to students' misuse or lack of use of the models provided in the activities. Certain items in the activity were designed such that the answer was explicitly stated in the model; therefore, these items were expected to elicit the lower Active engagement mode from student groups. However, observations showed students either did not use the model at all or used the model in an incomplete fashion, resulting in groups engaging at the higher engagement modes to generate the answer on their own. The second theme dealt with unfamiliar vocabulary. Groups engaged at higher-than-expected modes when unfamiliar scientific vocabulary was introduced in order to understand the meaning behind these terms. In this case, the mismatch in expected and observed engagement modes can create a positive effect on student learning. As students worked together and engaged at a higher mode to define the unfamiliar terms, they were expanding their scientific vocabulary, which is an important aspect of their growth. The third theme was specific to the Electronegativity and Polarity activity and related to students' proficiency in moving between different molecular representations. Students again displayed Interactive engagement although Active engagement was expected since the answer to the item was explicitly stated in the model. However, students struggled to relate Lewis structure representations with vector representations of bond dipoles. In addition, students had difficulty understanding how specific features of Lewis representations, e.g., lone electron pairs, were characterized in the vector representation.

This portion of the project evaluated the engagement of all group members and identified the engagement of the group as the highest mode of engagement demonstrated by any student during a conversation excerpt. However, it was noted that not all students engaged at the same mode; therefore, the next part of the project investigated the engagement of each student in the group.

RQ2. a) How do individual students' cognitive engagement vary while participating in small-group active learning activities in chemistry courses?

b) What factors may affect individual students' cognitive engagement?

Overall, individual students' engagement varied across three different observed activities in a General Chemistry class, and group size and timing of the activity during the term were identified as factors which had an effect on engagement. Analysis of group sizes which ranged from two to five students found that there is no single, "optimal" group size. Instead, results suggested that higher modes of engagement occurred with smaller groups or within subsets of larger groups. Furthermore, the higher engagement modes occurred when students with similar knowledge bases were grouped together regardless of group size.

Changes in engagement modes also occurred based on when during the term the activity was. During the first half of the term, students' engagement showed more variation; students had higher amounts of Interactive engagement and showed less variation across during the second half of the term. One possibility for this observation is that because General Chemistry I is the first term of college for many students, they may be figuring out what study behaviors benefit their learning, and this may result in fluctuations in their engagement. Later in the term, students may have established what behaviors work best for them and be less willing to change. However, the higher modes of engagement that were observed in the second half of the term occurred with different group sizes, suggesting that the effect on engagement may be a result of a combination of factors, i.e., similar knowledge bases and timing. In addition, students' opinion about group work may have influenced their engagement. Interviews with students confirmed this idea. For example, a student with a strong positive belief in the benefits of group work was more likely to engage at the Interactive mode than a student who had some reservations regarding the effectiveness of group work. Therefore, the stabilization of engagement observed during the second half of the term may be due to a variety of contributing factors. Another possibility for this trend is that the type of question being asked may influence engagement. Therefore, the relation between question type and engagement modes was explored further with the third research question.

RQ 3. What relations are observed between the type of question asked in the activities and students' level of cognitive engagement?

A statistical analysis using McNemar's test compared Constructive and Interactive engagement modes of individual students against algorithmic and explanation items on three different activities in a General Chemistry class. The results indicated a significant relation exists in the Solutions and Dilutions activity only. This activity consisted primarily of algorithmic items, and the significant relation was between these items and the Interactive mode. Analysis of student excerpts suggested that students demonstrated Interactive engagement on these items to resolve difficulties in associating variables with numerical values and determining the correct significant figures.

Finally, analysis of conversation excerpts in a Physical Chemistry class provided insight into the structure of the items themselves and their effect on student understanding, which was explored in the final research question.

Q4. a) How can analysis of group conversations inform improvements to learning activities to enhance student understanding?

b) What improvements can be made to learning activities to enhance student understanding?

Student group conversations during two Physical Chemistry activities (teaching concepts related to the Hydrogen Atom and Harmonic Oscillator models in quantum mechanics) were evaluated using cognitive load theory. Items where students struggled to complete the task or master the concept were identified, and the principles of scaffolding were applied to these items to reduce load. Scaffolding was used to break down complex items which required students to process and use multiple skills and concepts simultaneously into a series of simpler items which asked students to address each skill independently and then built up to the more complex item. Analysis of student groups using the new activities indicated that students' understanding improved and they struggled less.

Limitations

All research for this dissertation was conducted in a single term of a course (General Chemistry or Physical Chemistry) for a small sample size, i.e., only students who consented to participate in the study were part of the sample group. As such, the conclusions made cannot be generalized to a larger population of chemistry students. In addition, the ICAP framework assumes that certain behaviors signify specific engagement modes which may not always be accurate. Students may exhibit behaviors associated with a lower engagement mode while internally engaging at a higher mode. For example, a student may not show any evidence of generating new information and therefore would be coded as Active engagement even though they may be processing ideas which do result in the generation of new information (Constructive engagement). Furthermore, engagement has been defined as a multi-dimensional construct, and previous research has shown that there is conflation between the behavioral and cognitive dimensions (Fredricks *et al.*, 2004; Naibert and Barbera, 2022). It is also possible that factors within the emotional dimension may impact cognitive engagement. For example, if students do not have a positive sense of belonging in their group or class, this could affect their cognitive engagement.

The data used to identify engagement modes for the group as a whole was collected in an Honors General Chemistry class that was held remotely and no written artifacts were collected. Therefore, engagement modes were determined based only on the content of the conversation and written artifacts could not be used to corroborate these engagement modes. Additionally, the modality of the course may have affected engagement, as students may engage differently in the remote environment versus in person classes (Perets *et al.*, 2020).

Finally, groups did not remain consistent with regards to composition or size across multiple activities for the individual coding part of this project. Because students were placed in groups with new students for each activity, they may have engaged differently as they learned how to work together with different personalities.

Implications for Research

This research is a first step in understanding the role of cognitive engagement in group work. While observed trends in individual engagement have indicated relations between engagement and factors such group size and activity structure, it is likely that there are other factors which affect cognitive engagement. For example, previous research has shown that characteristics of the individual student, such as gender identity, students' aspirations, and academic capability, may also affect student engagement (Fullarton, 2002; Lee *et al.*, 2022). Therefore, additional studies focused on individual engagement while holding group size or composition constant would remove the potential conflation of these factors and may give insight into additional factors. Research into other models of group work, e.g., highly structured groups such as POGIL, or different type of activities, e.g., longer-term assignments such as problem-based learning, may also improve our understanding of students' cognitive engagement. In addition, student interviews highlighted the fact that student opinions of group work and their personal goals while working in a group may impact how they engage with other group members, and further investigation of this avenue could deepen our understanding of how students cognitively engage in group environments. To improve our understanding of how accurately ICAP identifies students' engagement modes, additional work could be done by using stimulated recall interviews where students can view and reflect on their behavior during group work. Finally, future work could expand on these initial results to model how both individual students' engagement and the factors that influence engagement affect learning outcomes.

Implications for Practice

Although the results of this dissertation are based on observations of a small number of students in two courses over a limited number of activities, there are still some valuable takeaways for practitioners. Analysis of expected versus observed group engagement modes identified areas of misalignments between what was intended in activities and what students did. Lack of use of models can result in students working towards an incorrect answer. In addition, analysis of the structure of the activities themselves indicated that providing clear models combined with scaffolded items helped guide students through the correct steps to solve the problem. Therefore, instructors may want to regularly discuss the importance of completely reading the model prior to answering items. Instructors may also benefit from monitoring group conversations as work through the activities progresses, and based on the direction of these conversations, they can provide targeted suggestions to effectively guide group problem-solving efforts. Monitoring these conversations can also provide instructors with insights into how students interact with the activity, and they may want to consider adapting aspects of the activities based on these insights.

A second area of misalignment involved scientific vocabulary. Although the use of unfamiliar terms resulted in students engaging at higher-than-expected modes, this can be a positive outcome. Part of an individual's growth in a professional field is becoming proficient with the technical language of that field. Therefore, instructors may want to consider how they can include scientific vocabulary in their course and activities in a productive manner with the goal of increasing students' knowledge.

Analysis of the engagement modes of individual students also provided some valuable takeaways for practitioners. Since students' engagement fluctuated during the first half of the term, this may be an opportunity for instructors to continually emphasize the benefits of group work and explicitly describe how participating in groups is most effective. For example, instructors may talk about what a productive versus an unproductive group conversation looks like. While the analysis of group size did not identify an "optimal" group size, the results did suggest that small group sizes are more likely to engage all participants as a single group. However, higher engagement modes were observed when students with similar levels of knowledge were grouped together regardless of group size. Therefore, although grouping students together based on knowledge level may not be feasible, instructors can form smaller groups whenever possible, and we suggest that instructors emphasize the importance and benefits of all students participating. Instructors can also specifically discuss the idea that each student brings a different idea to group, which may create a deeper understanding for all group members.

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Appendix A: Interview Guide

1. Tell me a little bit about why you are taking this class. Now I want to talk with you about the [NAME OF ACTIVITY] you recently completed.

2. Was any pre-work for this activity assigned?
    a. Did you complete it?

    b. What did the prework entail?

3. How much of this activity did you complete during the time allotted during class?

4. If any portion of the activity remained unfinished, did you complete it outside of class? On your own or with others?

5. Do you feel that this activity was successful?

    a. If so, how?

    b. Could things have gone better?

        i. If so, how?

6. Do you feel that the activity helped your understanding of the course material?

    a. If so, how do you think it helped?

    b. If not, why do you think it did not help?

7. Did the activity change your understanding of the course material?

    a. If yes/no, how or how did it not?

8. Could you provide specific examples of how your understanding may have or have not improved after participating in the activity?

9. Did you feel that working with your group during the activity helped your understanding of the material?

    a. If so, how do you think it helped?

    b. If not, why do you think it did not help?

Repeat question 10 and 11 for each model in the activity

10. Please glance through Model X and [key questions and/or exercises a-b] associated with it. Did you feel that any of the questions were more or less helpful or beneficial to your understanding of the material?

    a. If so, please explain why you chose this/these questions.

    b. If not, are there questions that you feel may have been helpful to your understanding of the material?

11. Did you notice more or less group conversations occurring with certain questions? If so, which?

    a. Why do you think there was more/less conversation?

12. Please look over Problems c-d. Did you feel that any of these questions were more or less helpful or beneficial to your understanding of the material?

    a. If so, please explain why you chose this/these questions.

    b. If not, are there questions that you feel may have been helpful to your understanding of the material?

13. Among the problems, did you notice more or less group conversations occurring with certain questions?

    a. If so, which?

    b. Why do you think there was more/less conversation?

14. Before concluding our discussion, do you have anything additional that you would like to share about the activity that we have not talked about yet?

Appendix B: Supporting Information for Chapter 5

SD-EX 4) What volume of the stock solution in Model 2 would you need to prepare 20.0 mL of a dilute solution with [$C_{12}H_{22}O_{11}$] = 0.1406 M?

1726 AMY: So you want the-

1727 TAMMY: The volume of the stock solution, right?

1728 AMY: Yeah. You need the volume of diluted. Is that V_D we're finding?

1729 TAMMY: So volume of the stock solution is gonna be concentrate cause of the Vc.

1730 AMY: Mm-hmm.

1731 TAMMY: Concentrated solution, and it says here, volume of the stock solution, right here on this side says Vc. (points to the model)

1732 AMY: Okay. Would you need to prepare 20? Oh, okay.

1733 TAMMY: Okay then.

1734 AMY: So we're solving for Vc.

1735 TAMMY: Solving for Vc. So then you wanna isolate the equation that way, right?

1736 AMY: Mm-hmm.

1737 TAMMY: So, and it already gives it right the back. What that is, right here. (points to equation in the model)

1738 AMY: Dang.

1739 TAMMY: So M_D…

1740 AMY: Alright, that's nice.

1741 TAMMY: M_D is V_D over Mc.

1742 AMY: Right, okay.

1743 TAMMY: Okay.

1744 MAI: So what would our Mc be?

1745 TAMMY: That is a good question. [TAMMY laughs]

1746 MAI: So are we using Model 2?

1747 AMY: Yeah.

1748 MAI: To like, we're gonna replace…Basically the top what I'm understanding and then we use 0.5625 as-, Uh, I'm sorry, my brain is moving too fast.

1749 AMY: Which one is which?

1750 TAMMY: Okay, so hold on. Oh, you want volume of the stock solution?

1751 AMY: Mm-hmm.

1752 TAMMY: Would you need to prepare 20 milliliters of the diluted solution-

1753 AMY: So that's-

1754 TAMMY: Of the molarity.

1755 AMY: Alright. So that's V_D and M_D that they give us.

1756 TAMMY: So molarity of the diluted solution is M_D.

1757 TAMMY: And then there's the molarity of the dilution. So the molarity is going to be 0.1406 M, okay?

1758 AMY: Yeah, yeah.

1759 TAMMY: That's that one. Okay. So that's M_D, then V_D volume of the dilute solution-

1760 AMY: That'd be the 20 milliliters, right?

1761 TAMMY: Okay. So 20 milliliters of that solution. That makes sense to me. Cause that's the volume of the dilute solution. Okay.

1762 AMY: So that means we just copy over the Mc.

1763 TAMMY: Right? What is the Mc?

1764 AMY: Oh cause it's a stock solution of .565 moles.

1765 TAMMY: Yeah. Yep, yep, yep, yep.

1766 AMY: That makes sense.

1767 TAMMY: That makes sense, so that is the stock solution. So Mc equals 0.5625 molarity. Okay. Then you just plug those in.

1768 AMY: And the unit should cancel that for-

1769 TAMMY: Yes. Yes. Absolutely. Yes. Um, we need to convert milliliters to liters.

1770 AMY: You're so right.

1771 TAMMY: Yes. You need to convert that cause otherwise, um, it's gonna be the wrong answer.

1772 AMY: Yeah.

1773 TAMMY: So I need to do that before, milliliters.

1774 MAI: Do we need to convert it to milliliters?

1775 TAMMY: Yes. Because molarity will always be moles over liters, always

1776 MAI: But we're not solving for molarity, we're solving for volume.

1777 AMY: Oh, you're right. So we only need milliliters, yeah.

1778 MAI: We don't need to convert that-

1779 AMY: Okay, and in the example they, they kept it as milliliters.

1780 TAMMY: Oh, all right. Thank you.

1781 AMY: Like one less step.

1782 TAMMY: Perfect. And then Mc is 0.5625. Perfect and then you just do math from there.

1783 AMY: Yeah.

1784 AMY: Did you get 4.999?

1785 ZOEY: Yeah but I'm thinking since it's a sig fig, or like do we need to do that?

1786 AMY: Oh yeah.

1787 TAMMY: Yep. How many sig figs would we have? Three.

1788 AMY: You're right. I was thinking the decimals.

1789 AMY: So 4.99.

1790 MAI: So, I was thinking cause it's like nine and nine, right?

1791 AMY: Oh.

1792 MAI: So would it be like five?

1793 ZOEY: 5.-

1794 TAMMY: 5.00?

1795 AMY: Yeah. Just throw in extra zeros to make it.

1796 MAI: Okay. So I just wanted to make sure.

Appendix C: Supporting Information for Chapter 6

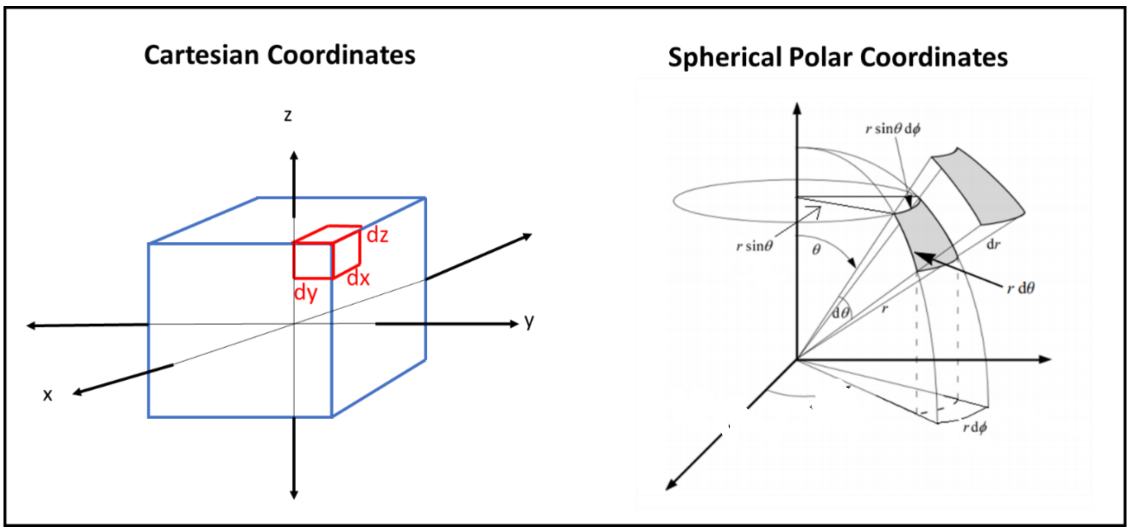
Hydrogen Atom Activity

(One Electron Atoms)

Goals:

- *To understand the relation between Cartesian and spherical polar coordinates*
    - *To identify the mathematical form of $d\tau$ and the integration limits in both coordinate systems*
- *To understand conceptually the components of the Hamiltonian for the hydrogen atom*
- *To be able to explain degeneracy and identify degenerate states*
- *To articulate the relation between quantum numbers and energy levels*
- *To understand the relation between ψ, quantum numbers, and orbitals*
- *To be able to evaluate average radius of an electron in the 1s orbital of the hydrogen atom*
- *To be able to calculate the most probable radius of an electron in the 1s orbital of the hydrogen atom*
- *To articulate what average and most probable radius represent conceptually*
    - *To be able to describe the difference between these two radii*

Model 1:



Questions 1 and 2 will help reinforce your understanding of the Cartesian and spherical polar coordinate systems. You will also be able to identify the volume element $d\tau$ and the limits of integration in both coordinate systems.

1. a) Write down the volume element $d\tau$ for the Cartesian coordinate system.

   b) What are the limits of integration over all space for the Cartesian coordinate system?

   c) Write down the volume element $d\tau$ for the spherical polar coordinate system.

   d) What are the limits of integration over all space for the spherical polar coordinate system?

2. a) Look at the integral below:

$$\iiint e^{-2r}\, cos^2\theta d\tau$$

   Does this integral use Cartesian or spherical polar coordinates?

   b) Evaluate the above integral over all space:

   These integrals may be helpful in solving this:

   $\int cos^2 ax\; dx = \frac{1}{2}x + \frac{1}{4a} sin2ax$

   $\int cos^m ax \sin ax\; dx = -\frac{(cos^{m+1} ax)}{(m+1)a}$

   $\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$

Model 2:

Hamiltonian for Hydrogen Atom

$$\hat{H} = \frac{-\hbar^2}{2\mu}\nabla^2 + \frac{-e^2}{4\pi\varepsilon_o r} \qquad \mu = \frac{m_p m_e}{m_p + m_e}$$

m_p: mass of proton = 1.67×10^{-27} kg
m_e: mass of electron = 9.11×10^{-31} kg

Questions 3 and 4 will help you to conceptually understand the individual terms in the Hamiltonian of the hydrogen atom.

3. a) Identify and write down the potential energy term in the Hamiltonian.

   b) What is the source of the potential energy in the hydrogen atom model?

4. a) This Hamiltonian contains a reduced mass term, μ. Calculate the reduced mass for a hydrogen atom.

   b) For the hydrogen atom, we typically replace μ with m_e in calculations. Based on your answer in part a, is this a valid assumption? Explain.

Model 3:

3-D Particle in a Box Solution (each side has length a)	Hydrogen Atom Solution
$\psi(x,y,z) = X(x)Y(y)Z(z)$	$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$
$E(n_x n_y n_z) = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$	$E_n = -\frac{\hbar^2}{2m_e n^2 a_o^2}$
Three principal quantum numbers: n_x, n_y, n_z n_x, n_y, n_z *= 1, 2, 3, … ∞*	*Principal quantum number: n = 1, 2, 3, … ∞* *Azimuthal quantum number l = 0, 1, 2, … n-1* *Magnetic quantum number* m_l *= -l, -l+1, -l+2, … l-1, l*

Questions 5-10 will help you apply the quantum number rules to understand the definition of degeneracy and to be able to identify degenerate states. You will also understand how quantum numbers relate to energy.

5. Are the following hydrogen atom wavefunctions (ψ_{n,l,m_l}) allowed? Use the quantum number rules to explain your reasoning.

   a) $\psi_{1,0,0}$

   b) $\psi_{1,-1,0}$

   c) $\psi_{4,3,-1}$

   d) $\psi_{0,0,0}$

6. Is it possible for the energy of the hydrogen atom to be zero? If not, why not? If so, under what conditions?

7. a) Identify the value of the quantum numbers and the associated wavefunction corresponding to the ground state (lowest energy state) of an electron using the ***3-dimensional particle in a box model.***

   b) Write the energy expression for the ground state of an electron using the 3-dimensional particle in a box model.

8. a) Identify the value of the quantum numbers corresponding to the ground state (lowest energy state) of a ***hydrogen atom.***

   b) Write the energy expression for the ground state of a hydrogen atom.

9. a) Write down the quantum numbers for the three possible wavefunctions (n, l, m_l) for the <u>first excited state</u> of an ***electron using the 3-dimensional particle in a box model***.

   b) Write down the energy expressions for each wavefunction.

c) What can you say about the energy states of the wavefunctions you determined in 9b?

d) Are these wavefunctions degenerate? Use the definition of degeneracy to explain your answer.

10. Use the following steps to write down the quantum numbers for all possible wavefunctions for the <u>first excited state</u> of a ***hydrogen atom***.

a) What is n for the first excited state?

b) What are the possible values of l for the first excited state?

c) What are the possible values of m_l for each value of l noted in 10b?

d) Using your responses from 10a-c, write down all the possible wavefunctions.

e) Write out the energy term of each wavefunction and determine whether or not these energy states are degenerate.

Questions 11-15 are designed to help you interpret the quantum numbers n, l, m_l *conceptually.*

11. The energy expression for the hydrogen atom in Model 3 can be re-written as:

$$E_n = -\frac{\hbar^2}{2m_e a_o^2} \cdot \frac{1}{n^2}$$

a) What term(s) in this expression can change?

b) Write the energy expression for an electron at n = 2 and n = 3.

c) Given that the principal quantum number (n) reflects the average relative distance between the electron and the nucleus, describe what is happening to the energy with increasing n.

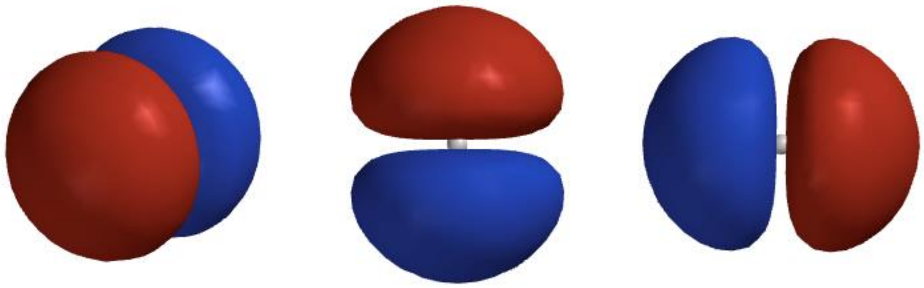
12. a) Explain ionization energy in terms of the quantized energy levels of the hydrogen atom model. (Hint: what is happening to the electron during ionization?)

b) Is the ionization energy greater for a hydrogen atom in the state $\psi_{2,1,0}$ or $\psi_{4,3,2}$? Explain.

13. The images below represent the probability distribution of an electron with azimuthal quantum number (l) equal to zero and one. What concept or idea from General Chemistry do the azimuthal quantum numbers correspond to?

i. $l = 0$

ii. $l = 1$



14. a) How many possible magnetic quantum numbers (m_l) are there when $l = 0$?

b) How many possible magnetic quantum numbers (m_l) are there when $l = 1$?

c) Given your answers to parts a and b as well as question 13, how might you describe what the m_l quantum number corresponds to?

Model 4:

Operator $\hat{r} \rightarrow r \cdot f(r)$

General Form of Hydrogen Atom Solution

$$\psi_{n,l,m_l} = R_{n,l}(r) Y_{l,m_l}(\theta, \phi)$$

Average value Theorem

$$\langle \hat{\alpha} \rangle = \frac{\int^{all\ space} \psi^* \hat{\alpha}\, \psi d\tau}{\int^{all\ space} \psi^* \psi d\tau}$$

Solution for the 1s electron
$(\boldsymbol{n = 1, l = 0, m_l = 0})$

$$\psi_{1,0,0} = R_{1,0}(r) Y_{0,0}(\theta, \phi)$$

$$R_{1,0}(r) = 2({}^{1}/_{a_o})^{3/2} e^{-\frac{r}{a_o}}$$

$$Y_{0,0}(\theta, \phi) = ({}^{1}/_{4\pi})^{1/2}$$

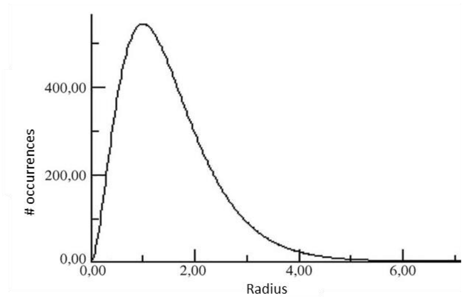


Figure 1: Distribution of the Radius of the Hydrogen Atom in the 1s orbital state

Questions 15-19 are intended to help you understand conceptually and mathematically what average and most probable radius mean.

15. a) Is $\psi_{1,0,0}$ an eigenfunction of the operator r?

b) Recall that when a wavefunction is NOT an eigenfunction of an operator, then a measurement of the property of the operator gives a range of values. Figure 1 (Model 4) plots the results of many measurements of the radius of the hydrogen atom in the 1s orbital state. What concept from quantum mechanics does this correspond to?

c) Using Figure 1, what radius would be measured most frequently?

We can see from question 15 that not all radii are equally probable. Therefore, an average radius must be weighted to account for this distribution. Question 16 will walk you through the mathematical steps to determine the average radius of the hydrogen atom in the 1s orbital state.

16. a) Use the average value theorem and the wave functions in Model 4 to write out the expression for the average radius of the hydrogen atom in the 1s orbital state. Make sure your expression includes the limits of integration for each variable.

b) Recall that the expression in the denominator, $\int^{all\ space} \psi^* \psi d\tau$, is the probability of the electron being present over all space and determines the normalization constant. If the function is normalized, this expression equals 1. $\psi_{1,0,0}$ has already been normalized. (You can prove this to yourself if you choose). Given this information, simplify the expression for average radius from part a.

c) Separate the radial and angular components (collect terms by like variables, i.e., collect all r terms together, all θ terms, etc).

d) Evaluate the angular components from part c. What does your result tell you?

e) Evaluate your simplified expression to determine the average radius of the hydrogen atom in the 1s orbital state.

Challenge Problem:

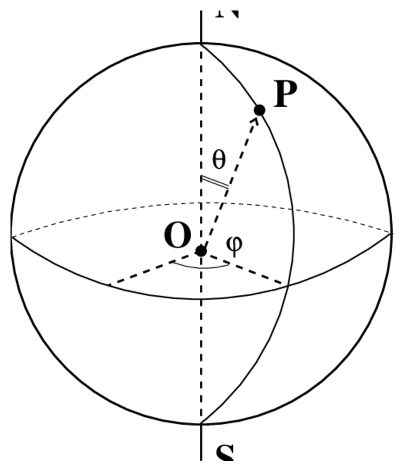
17. Define the most probable radius of the hydrogen atom in the 1s orbital state.

18. This question takes you through steps to determine the most probable radius of the hydrogen atom in the 1s orbital state.

a) Write the general expression for the probability density of the electron.

b) The *radial* probability density is the probability of the electron being at a specific radius r. Write down the expression for the radial probability density.

c) Consider the diagram of a sphere below. Is the magnitude of the radius to any point on the sphere affected by the angular components θ and ϕ?



d) Since the s orbital is spherical, the electron could be located at any point in a shell of radius r. Write an expression for the area of this shell.

e) Using your answers in parts a-d, write an expression for the ***total*** probability density of an electron at radius r.

f) Using Figure 1, how would you mathematically determine the most probable radius?

g) Calculate the partial derivative with respect to r of the probability density expression.

h) Use your answers in parts f and g to determine the most probable radius of the hydrogen atom in the 1s orbital state.

19. Taking into account the values of the average and most probable radius from questions 16 and 18, give an explanation for the difference in these values.

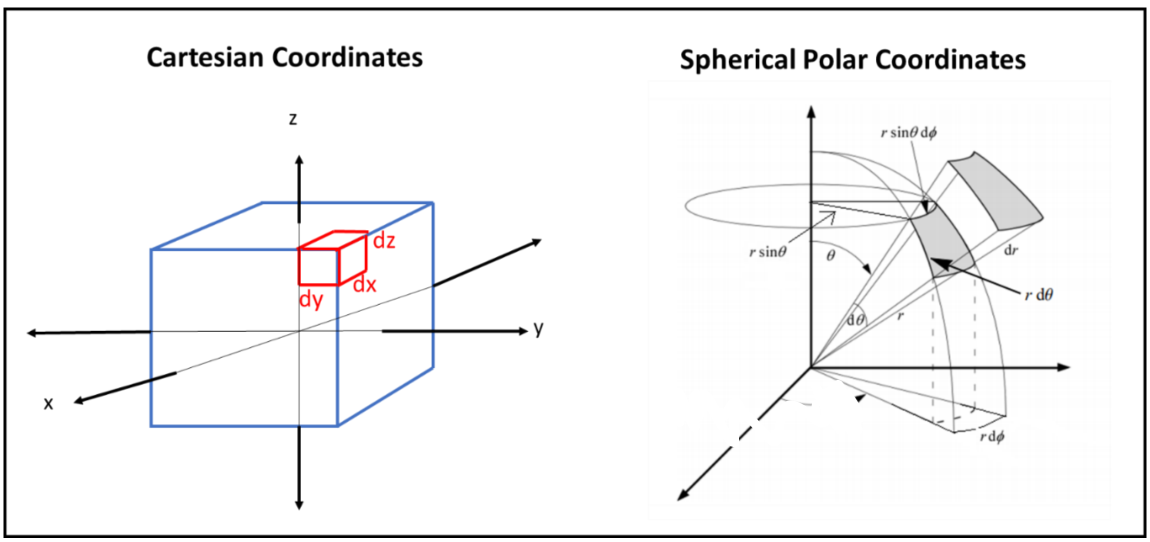
Hydrogen Atom Activity – KEY

(One Electron Atoms)

Goals:

- *To understand the relation between Cartesian and spherical polar coordinates*
    - *To identify the mathematical form of $d\tau$ and the integration limits in both coordinate systems*
- *To understand conceptually the components of the Hamiltonian for the hydrogen atom*
- *To be able to explain degeneracy and identify degenerate states*
- *To articulate the relation between quantum numbers and energy levels*
- *To understand the relation between ψ, quantum numbers, and orbitals*
- *To be able to evaluate average radius of an electron in the 1s orbital of the hydrogen atom*
- *To be able to calculate the most probable radius of an electron in the 1s orbital of the hydrogen atom*
- *To articulate what average and most probable radius represent conceptually*
    - *To be able to describe the difference between these two radii*

Model 1:



Questions 1 and 2 will help reinforce your understanding of the Cartesian and spherical polar coordinate systems. You will also be able to identify the volume element $d\tau$ and the limits of integration in both coordinate systems.

1. a) Write down the volume element $d\tau$ for the Cartesian coordinate system.

$$d\tau = dx\,dy\,dz$$

b) What are the limits of integration over all space for the Cartesian coordinate system?

The limits of integration are $-\infty$ to $+\infty$ for x, y, and z.

c) Write down the volume element $d\tau$ for the spherical polar coordinate system.

$$d\tau = r^2 sin\theta\, dr\, d\theta\, d\phi$$

d) What are the limits of integration over all space for the spherical polar coordinate system?

The limits of integration are:

Zero to ∞ for r

Zero to π for θ

Zero to 2π for ϕ

2. a) Look at the integral below:

$$\iiint e^{-2r}\, cos^2\theta d\tau$$

Does this integral use Cartesian or spherical polar coordinates?

This integral has r and θ. Therefore, it is in spherical polar coordinates.

b) Evaluate the above integral over all space:

These integrals may be helpful in solving this:

$\int cos^2ax\, dx = \frac{1}{2}x + \frac{1}{4a}sin2ax$

$\int cos^m ax \sin ax\, dx = -\frac{(cos^{m+1}ax)}{(m+1)a}$

$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} e^{-2r}cos^2\theta\, r^2 sin\theta\, dr\, d\theta\, d\phi$$
$$= \int_0^{2\pi} d\phi \int_0^{\pi} cos^2\theta\, sin\theta\, d\theta \int_0^{\infty} r^2 e^{-2r} dr$$

$$= [2\pi]\left[\frac{-cos\theta}{3}\right]_0^{\pi}\int_0^{\infty} r^2 e^{-2r} dr = [2\pi]\left[\frac{2}{3}\right]\left[\frac{2!}{2^3}\right] = \boldsymbol{\frac{\pi}{3}}$$

Model 2:

Hamiltonian for Hydrogen Atom

$$\hat{H} = \frac{-\hbar^2}{2\mu}\nabla^2 + \frac{-Ze^2}{4\pi\varepsilon_o r} \qquad \mu = \frac{m_p m_e}{m_p + m_e}$$

m_p: mass of proton = 1.67 x 10^{-27} kg
m_e: mass of electron = 9.11 x 10^{-31} kg

Questions 3 and 4 will help you to conceptually understand the individual terms in the Hamiltonian of the hydrogen atom.

3. a) Identify and write down the potential energy term in the Hamiltonian.

   The potential energy term is:

$$\frac{-Ze^2}{4\pi\varepsilon_o r}$$

   b) What is the source of the potential energy in the hydrogen atom model?

   The potential energy term comes from the Coulombic attraction between the proton and electron in the hydrogen atom.

4. a) This Hamiltonian contains a reduced mass term, μ. Calculate the reduced mass for a hydrogen atom.

$$\mu = \frac{m_p m_e}{m_p + m_e} = \frac{(1.67 \times 10^{-27} kg)(9.11 \times 10^{-31} kg)}{(1.67 \times 10^{-27} kg) + (9.11 \times 10^{-31} kg)}$$

$$= \mathbf{9.11 \times 10^{-31} kg}$$

   b) For the hydrogen atom, we typically replace μ with m_e in calculations. Based on your answer in part a, is this a valid assumption? Explain.

   Yes, it is a valid assumption. Since the calculated value of the reduced is equal to the mass of the electron (to 2 significant figures), it is valid to make this assumption.

Model 3:

3-D Particle in a Box Solution (each side has length a)	**Hydrogen Atom Solution**
$\psi(x,y,z) = X(x)Y(y)Z(z)$	$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$
$E(n_x n_y n_z) = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$	$E_n = -\frac{Z^2\hbar^2}{2m_e n^2 a_o^2}$
Three principal quantum numbers: n_x, n_y, n_z *n_x, n_y, n_z = 1, 2, 3, ... ∞*	*Principal quantum number: n = 1, 2, 3, ... ∞* *Azimuthal quantum number l = 0, 1, 2, ... n-1* *Magnetic quantum number m_l = -l, -l+1, -l+2, ... l-1, l*

Questions 5-10 will help you apply the quantum number rules to understand the definition of degeneracy and to be able to identify degenerate states. You will also understand how quantum numbers relate to energy.

5. Are the following hydrogen atom wavefunctions (ψ_{n,l,m_l}) allowed? Use the quantum number rules to explain your reasoning.

a) $\psi_{1,0,0}$

Yes, this is allowed. *n, l, m_l* all follow the quantum number rules.

b) $\psi_{1,-1,0}$

No, this is not allowed. *l* cannot be a negative value.

c) $\psi_{4,3,-1}$

Yes, this is allowed. *n, l, m_l* all follow the quantum number rules.

d) $\psi_{0,0,0}$

No, this is not allowed. *n* cannot equal zero.

6. Is it possible for the energy of the hydrogen atom to be zero? If not, why not? If so, under what conditions?

   No, this is not possible. Since $E = -\frac{Z^2\hbar^2}{2m_e n^2 a_0^2}$ and the lowest value for *n* is 1, and all other values in the expression are non-zero, the energy of the hydrogen atom can never be zero.

7. a) Identify the value of the quantum numbers corresponding to the ground state (lowest energy state) of an electron using the ***3-dimensional particle in a box model.***

   $$The\ ground\ state\ would\ be\ when\ n_x = n_y = n_z = 1$$

   b) Write the energy expression for the ground state of an electron using the 3-dimensional particle in a box model.

   $$E_{1,1,1} = \frac{h^2}{8ma^2}(3) = \boldsymbol{\frac{3h^2}{8ma^2}}$$

8. a) Identify the value of the quantum numbers corresponding to the ground state (lowest energy state) of a ***hydrogen atom.***

   $$The\ ground\ state\ would\ be\ when\ n = 1, l = 0, m_l = 0$$

b) Write the energy expression for the ground state of a hydrogen atom.

$$E_1 = -\frac{(1^2)\hbar^2}{2m_e(1)^2 a_o^2} = -\boldsymbol{\frac{\hbar^2}{2m_e a_o^2}}$$

9. a) Write down the quantum numbers (n, l, m_l) of the three possible wavefunctions for the <u>first excited state</u> of an electron using the ***3-dimensional particle in a box model***.

$The\ first\ excited\ state\ would\ be\ when\ n_x\ or\ n_y\ or\ n_z = 2\ and\ the\ other\ two\ are\ equal\ to\ 1.$

$2, 1, 1 \qquad\qquad 1, 2, 1 \qquad\qquad 1, 1, 2$

b) Write down the energy expressions for each wavefunction.

$$\psi_{2,1,1} \rightarrow (2^2 + 1^2 + 1^2) = \frac{6h^2}{8ma^2} = \boldsymbol{\frac{3h^2}{4ma^2}}$$

$$\psi_{1,2,1} \rightarrow \frac{h^2}{8ma^2}(1^2 + 2^2 + 1^2) = \frac{6h^2}{8ma^2} = \boldsymbol{\frac{3h^2}{4ma^2}}$$

$$\psi_{1,1,2} \rightarrow \frac{h^2}{8ma^2}(1^2 + 1^2 + 2^2) = \frac{6h^2}{8ma^2} = \boldsymbol{\frac{3h^2}{4ma^2}}$$

c) What can you say about the energy states of the wavefunctions you determined in 9b?

The energy states of all three wavefunctions are the same.

d) Are these wavefunctions degenerate? Use the definition of degeneracy to explain your answer.

Yes. If multiple wavefunctions (i.e., electrons) have the same energy, that energy state is degenerate.

10. Use the following steps to write down the quantum numbers for all possible wavefunctions for the first excited state of a ***hydrogen atom***.

a) What is n for the first excited state?

$$The\ first\ excited\ state\ would\ be\ when\ n = 2$$

b) What are the possible values of l for the first excited state?

$In\ the\ first\ excited\ state, l = 0\ and\ l = 1$

c) What are the possible values of m_l for each value of l noted in 10b?

$For\ l = 0, m_l = 0.$

$For\ l = 1, m_l = -1, 0, and\ 1.$

d) Using your responses from 10a-c, write down all the possible sets of quantum numbers.

$2, 0, 0$	$2, 1, 0$
$2, 1, 1$	$2, 1, -1$

e) Write out the energy term of each wavefunction and determine whether or not these energy states are degenerate.

$n = 2$ for all four wavefunctions. Therefore, for all functions

$$E_2 = -\frac{\hbar^2}{8m_e a_o^2}$$

All four wavefunctions have the same n and therefore fill the same energy state. The energy states for the first excited state of the hydrogen atom are degenerate.

Questions 11-15 are designed to help you interpret the quantum numbers n, l, m_l conceptually.

11. The energy expression for the hydrogen atom in Model 3 can be re-written as:

$$E_n = -\frac{\hbar^2}{2m_e a_o^2} \cdot \frac{1}{n^2}$$

a) What term(s) in this expression can change?

Only the $\frac{1}{n^2}$ term changes. All other terms remain constant.

b) Write the energy expression for an electron at n = 2 and n = 3.

$$For\ n = 2{:}\ \boldsymbol{E_2} = -\frac{\boldsymbol{\hbar^2}}{\boldsymbol{2m_e a_o^2}} \cdot \frac{\boldsymbol{1}}{\boldsymbol{4}}$$

$$For\ n = 3{:}\ \boldsymbol{E_3} = -\frac{\boldsymbol{\hbar^2}}{\boldsymbol{2m_e a_o^2}} \cdot \frac{\boldsymbol{1}}{\boldsymbol{9}}$$

c) Given that the principal quantum number (n) reflects the average relative distance between the electron and the nucleus, describe what is happening to the energy with increasing n.

As n increases, meaning the average relative distance between the electron and nucleus increase, the energy of the hydrogen atom is decreasing. This makes sense since part of the energy is the Coulombic attraction to the nucleus (see the Hamiltonian) which will decrease as the electron is further from the nucleus.

12. a) Explain ionization energy in terms of the quantized energy levels of the hydrogen atom model. (Hint: what is happening to the electron during ionization?)

Ionization energy is the energy to remove the electron from the atom. Since increasing the quantum number *n* suggests that the relative distance between the electron and nucleus is increasing, an infinitely high *n* would mean that the electron has been removed from the atom. Since $E\ \alpha \frac{1}{n^2}$, at an infinitely high n, $E_\infty = 0$. Therefore, the energy to remove the electron at some specified E_n from the atom (ionization energy) would be $E_\infty - E_n = -E_n$.

b) Is the ionization energy greater for a hydrogen atom in the state $\psi_{2,1,0}$ or $\psi_{4,3,2}$? Explain.

$$For\ \psi_{2,1,0}: n = 2, E_2 = -\frac{1}{4}\frac{\hbar^2}{2m_e a_o^2}\ and\ the\ ionization\ energy\ is\ \frac{1}{4}\frac{\hbar^2}{2m_e a_o^2}$$

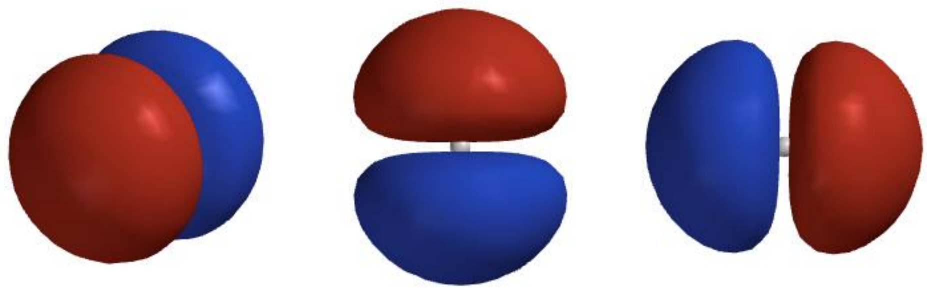
$$For\ \psi_{4,3,2}: n = 4, E_4 = -\frac{1}{16}\frac{\hbar^2}{2m_e a_o^2}\ and\ the\ ionization\ energy\ is\ \frac{1}{16}\frac{\hbar^2}{2m_e a_o^2}$$

The ionization energy for the electron at $n = 2$ is greater. This makes sense since the $n = 2$ electron is closer to the nucleus than the $n = 4$ electron and would require more energy to remove it from the atom.

13. The images below represent the probability distribution of an electron with azimuthal quantum number (l) equal to zero and one. What concept or idea from General Chemistry do the azimuthal quantum numbers correspond to?

iii. $l = 0$

iv. $l = 1$



The shapes of these probability distributions are the same as the s and p orbitals from General Chemistry. Therefore, the azimuthal quantum number corresponds to the shape of the region of space occupied by an electron.

14. a) How many possible magnetic quantum numbers (m_l) are there when $l = 0$?

When $l = 0$, there is only one possible value for $m_l = 0$.

b) How many possible magnetic quantum numbers (m_l) are there when $l = 1$?

When $l = 1$, m_l has three possible values: -1, 0, and 1.

c) Given your answers to parts a and b as well as question 13, how might you describe what the m_l quantum number corresponds to?

Since l represents the different orbital types ($l = 0$ for the s orbital and $l = 1$ for the p orbital), and there is one m_l value for the s orbital and three m_l values for the p orbital, this corresponds to the orbital orientations. Since the s orbital is a sphere, there is only one orientation. However, the p orbitals have three equivalent (degenerate) orbitals, each oriented in a different direction (x, y, and z).

Model 4:

Operator $\hat{r} = r \cdot f(r)$

General Form of Hydrogen Atom Solution

$$\psi_{n,l,m_l} = R_{n,l}(r)Y_{l,m_l}(\theta,\phi)$$

Solution for the 1s electron
($n = 1, l = 0, m_l = 0$)

$$\psi_{1,0,0} = R_{1,0}(r)Y_{0,0}(\theta,\phi)$$

$$R_{1,0}(r) = 2(Z/a_o)^{3/2}e^{-\frac{Zr}{a_o}}$$

$$Y_{0,0}(\theta,\phi) = (1/4\pi)^{1/2}$$

Average value Theorem

$$\langle\hat{\alpha}\rangle = \frac{\int^{all\ space}\psi^*\hat{\alpha}\,\psi d\tau}{\int^{all\ space}\psi^*\psi d\tau}$$

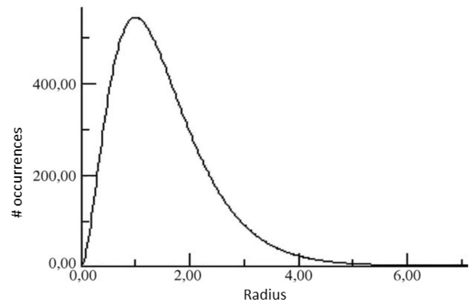


Figure 1: Distribution of the Radius of the Hydrogen Atom in the 1s orbital state

Questions 15-19 are intended to help you understand conceptually and mathematically what average and most probable radius mean.

15. a) Is $\psi_{1,0,0}$ an eigenfunction of the operator r?

No, it is not an eigenfunction because $r \cdot \psi_{1,0,0}$ does not give a constant value.

b) Recall that when a wavefunction is NOT an eigenfunction of an operator, then a measurement of the property of the operator gives a range of values. Figure 1 (Model 4) plots the results of many measurements of the radius of the hydrogen atom in the 1s orbital state. What concept from quantum mechanics does this correspond to?

This plot is the same as a probability distribution in quantum mechanics.

c) Using Figure 1, what radius would be measured most frequently?

From Figure 1, the highest number of occurrences is at a radius of 1.

We can see from question 15 that not all radii are equally probable. Therefore, an average radius must be weighted to account for this distribution. Question 16 will walk you through the mathematical steps to determine the average radius of the hydrogen atom in the 1s orbital state.

16. a) Use the average value theorem and the wave functions in Model 4 to write out the expression for the average radius of the hydrogen atom in the 1s orbital state. Make sure your expression includes the limits of integration for each variable.

Note that $\psi^* = \psi$ for this wavefunction

$$\langle \hat{r} \rangle = \frac{\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{1,0}^*(r)Y_{0,0}^*(\theta,\phi)\, r\, R_{1,0}(r)Y_{0,0}(\theta,\phi)\, r^2\, sin\theta\, dr\, d\theta\, d\phi}{\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{1,0}^*(r)Y_{0,0}^*(\theta,\phi)\, R_{1,0}(r)Y_{0,0}(\theta,\phi)\, r^2\, sin\theta\, dr\, d\theta\, d\phi}$$

$$\langle \hat{r} \rangle = \frac{\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} 2(1/a_o)^{3/2} e^{-\frac{r}{a_o}} (1/4\pi)^{1/2}\, r\, 2(1/a_o)^{3/2} e^{-\frac{r}{a_o}} (1/4\pi)^{1/2}\, r^2\, sin\theta\, dr\, d\theta\, d\phi}{\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} 2(1/a_o)^{3/2} e^{-\frac{r}{a_o}} (1/4\pi)^{1/2}\, 2(1/a_o)^{3/2} e^{-\frac{r}{a_o}} (1/4\pi)^{1/2}\, r^2\, sin\theta\, dr\, d\theta\, d\phi}$$

$$\boldsymbol{\langle \hat{r} \rangle = \frac{\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} 4(1/a_o)^3 e^{-\frac{2r}{a_o}} (1/4\pi)\, r^3\, sin\theta\, dr\, d\theta\, d\phi}{\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} 4(1/a_o)^3 e^{-\frac{2r}{a_o}} (1/4\pi)\, r^2\, sin\theta\, dr\, d\theta\, d\phi}}$$

b) Recall that the expression in the denominator, $\int^{all\ space} \psi^* \psi d\tau$, is the probability of the electron being present over all space and determines the normalization constant. If the function is normalized, this expression equals 1. $\psi_{1,0,0}$ has already been normalized. (You can prove this to yourself if you choose). Given this information, simplify the expression for average radius from part a.

$$\langle \hat{r} \rangle = \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} 4\left(\frac{1}{a_o}\right)^3 e^{-\frac{2r}{a_o}} \left(\frac{1}{4\pi}\right) r^3 sin\theta\ dr\ d\theta\ d\phi$$

c) Separate the radial and angular components (collect terms by like variables, i.e., collect all r terms together, all θ terms, etc).

$$\langle \hat{r} \rangle = \left[\left(\frac{1}{4\pi}\right) \int_0^{2\pi} d\phi \int_0^{\pi} sin\theta\ d\theta \right] \left[4\left(\frac{1}{a_0}\right)^3 \int_0^{\infty} r^3\, e^{-\frac{2r}{a_o}}\, dr \right]$$

d) Evaluate the angular components from part c. What does your result tell you?

$$\left(\frac{1}{4\pi}\right) \int_0^{2\pi} d\phi \int_0^{\pi} sin\theta\ d\theta = \left(\frac{1}{4\pi}\right)[2\pi][-\cos\theta]_0^{\pi} = \left(\frac{1}{4\pi}\right)[2\pi][1-(-1)] = \mathbf{1}$$

Because this integral is equal to one, we know that the angular components are normalized.

e) Evaluate your simplified expression to determine the average radius of the hydrogen atom in the 1s orbital state.

$$\langle\hat{r}\rangle = 4\left({}^{1}/_{a_0}\right)^3 \int_0^\infty r^3\, e^{-\frac{2r}{a_o}}\, dr$$

$$\langle\hat{r}\rangle = {}^{4}/_{a_o^3} \int_0^\infty r^3\, e^{-\frac{2r}{a_o}}\, dr$$

$$\langle\hat{r}\rangle = {}^{4}/_{a_o^3} \int_0^\infty r^3\, e^{-\frac{2r}{a_o}}\, dr$$

Using the integral tables:

$$\langle\hat{r}\rangle = {}^{4}/_{a_o^3}\left[\frac{3!}{\left({}^{2}/_{a_o}\right)^4}\right] = \left({}^{4}/_{a_o^3}\right)\left({}^{6a_o^4}/_{16}\right) = \boldsymbol{\frac{3}{2}a_o}$$

<u>Challenge Problem:</u>

17. Define the most probable radius of the hydrogen atom in the 1s orbital state.

This is the radial position where the electron is most likely to be.

18. This question takes you through steps to determine the most probable radius of the hydrogen atom in the 1s orbital state.

a) Write the general expression for the probability density of the electron.

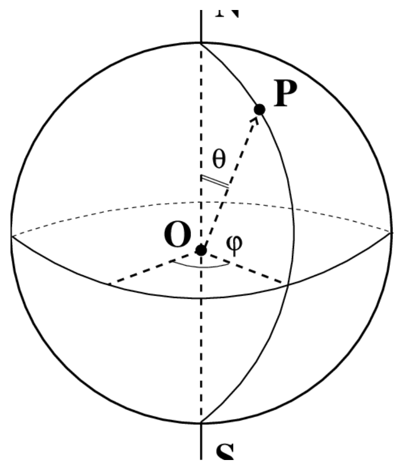
The probability density expression is $\psi^*\psi$.

Recall that for this wavefunction $\psi^* = \psi$.

b) The *radial* probability density is the probability of the electron being at a specific radius r. Write down the expression for the radial probability density.

Radial probability density = $R^*R = 2\left(1/a_o\right)^{3/2} e^{-\frac{r}{a_o}}\, 2\left(1/a_o\right)^{3/2} e^{-\frac{r}{a_o}} =$ $\boldsymbol{\left(4/a_o^3\right) e^{-\frac{2r}{a_o}}}$

c) Consider the diagram of a sphere below. Is the magnitude of the radius to any point on the sphere affected by the angular components θ and ϕ?



No, the magnitude of the radius will be the same for any point on the sphere. Therefore, the values of θ and ϕ will not affect the magnitude of r.

d) Since the s orbital is spherical, the electron could be located at any point in a shell of radius r. Write an expression for the area of this shell.

$4\pi r^2$

e) Using your answers in parts a-d, write an expression for the ***total*** probability density of an electron at radius r.

$$\psi^*\psi\, 4\pi r^2 = R^*R\, 4\pi r^2 = \boldsymbol{\left(4/a_o^3\right) e^{-\frac{2r}{a_o}}\, 4\pi r^2}$$

f) Using Figure 1, how would you mathematically determine the most probable radius?

You can determine the most probable radius by determining where the maximum is. This can be done by calculating the derivative and setting it equal to zero.

g) Calculate the partial derivative with respect to r of the probability density expression.

$$R^*R = 2\left({}^{1}/{}_{a_o}\right)^{3/2} e^{-\frac{r}{a_o}}\, 2\left({}^{1}/{}_{a_o}\right)^{3/2} e^{-\frac{r}{a_o}} = \left({}^{4}/{}_{a_o^3}\right) e^{-\frac{2r}{a_o}}$$

Remember to include the $4\pi r^2$ term to account for the surface area of the atom:

$$\frac{\partial}{\partial r}\left({}^{4}/{}_{a_o^3}\right) e^{-\frac{2r}{a_o}}(\,4\pi r^2) = \frac{\partial}{\partial r}\left[\frac{16\pi}{a_o^3}\left(r^2 e^{-\frac{2r}{a_o}}\right)\right]$$

Using the Chain Rule:

$$= \frac{16\pi}{a_o^3}\left[\,2re^{-\frac{2r}{a_o}} + r^2\left(-\frac{2}{a_o}\right)e^{-\frac{2r}{a_o}}\right]$$

h) Use your answers in parts f and g to determine the most probable radius of the hydrogen atom in the 1s orbital state.

$$\frac{16\pi}{a_o^3}\left[\,2re^{-\frac{2r}{a_o}} + r^2\left(-\frac{2}{a_o}\right)e^{-\frac{2r}{a_o}}\right] = 0$$

$$\left[\,2re^{-\frac{2r}{a_o}} + r^2\left(-\frac{2}{a_o}\right)e^{-\frac{2r}{a_o}}\right] = 0$$

$$e^{-\frac{2r}{a_o}}\left(2r - \frac{2r^2}{a_o}\right) = 0$$

$$\left(2r - \frac{2r^2}{a_o}\right) = 0$$

$$2r\left(1 - \frac{r}{a_o}\right) = 0$$

$$\frac{r}{a_o} = 1$$

$$\boldsymbol{r = a_o \; Most\ probable\ radius}$$

19. Taking into account the values of the average and most probable radius from questions 16 and 18, give an explanation for the difference in these values.

The average radius is $\frac{3}{2}a_o$, and the most probable radius is a_o. This difference is because the average radius takes into account all possible radial positions that the electron can occupy and the probability at each of these radii. This means that the average radius is really a *weighted* average. The most probable radius is a single radius where the electron is most likely to occur.

<u>Harmonic Oscillator Worksheet</u>

<u>Prior Knowledge:</u>

These questions are to help you review information you have learned previously and will be helpful in this activity.

1. a) What is the mathematical relation between wavelength (λ) and frequency (υ)?

   b) What are the units of each variable?

2. a) Describe in your own words how wavenumber relates to wavelength and frequency and provide an equation showing the relation. (Note that although chemists refer to IR “frequencies”, these numbers are actually reported in units of *wavenumbers*).

   b) What are the units for wavenumber ($\tilde{\upsilon}$)?

3) The Newton (N) is a derived unit composed of SI base units. Break down the Newton into its component units.

Goals:

- *To recognize that the quantum harmonic oscillator provides a model for the quantized vibrational energy of diatomic molecules*
    - *To recognize that wavelength, frequency, and wavenumber are all used as different representations of energy*
    - *To understand the influence of reduced mass on the magnitude of a vibrational frequency*
- *To articulate how the relation between force constant and frequency allows for the identification of molecules through infrared spectroscopy*
- *To use knowledge of vibrational energy levels to explain IR spectra*

Harmonic Oscillator Model

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \qquad E = \left(n + \frac{1}{2}\right)h\upsilon$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \qquad h = 6.626\ x\ 10^{-34}\ J \cdot s$$

Key Questions

1. What is the relation between reduced mass (μ) and frequency? Describe in your own words.

2. What is the relation between force constant (k) and frequency? Describe in your own words.

3. A $C - N$ single bond, $C = N$ double bond, and $C \equiv N$ triple bond will have IR frequencies at roughly 1100 cm^{-1}, 1660 cm^{-1}, and 2220 cm^{-1}, respectively. Use your knowledge of the relation between frequency and force constant to match each force constant to its corresponding C-N bond. NO CALCULATION NECESSARY!

1. $C \equiv N$	A. 1047.6 N/m
2. $C = N$	B. 1873.7 N/m
3. $C - N$	C. 460.0 N/m

Exercises

4. a) Calculate the reduced mass of a **single** hydrogen *molecule*. Include units in your answer. (molar mass of hydrogen = 1.008 g/mol). Report your answer in kilograms.

b) Calculate the reduced mass of a **single** deuterium *molecule*. Include units in your answer. (molar mass of deuterium = 2.014 g/mol). Report your answer in kilograms.

5. a) Compare the values you calculated for the reduced mass of the hydrogen and deuterium molecules. What do you notice?

b) The IR frequencies of hydrogen and deuterium are 4159.5 cm^{-1} and 2990.3 cm^{-1}, respectively. Calculate the force constants for a hydrogen and deuterium molecule. Force constants should be reported in units of N/m.

c) Compare the values you calculated for the force constants of the hydrogen and deuterium molecules. What do you notice?

d) Based on the harmonic oscillator model and your calculated values for reduced mass and force constants, what variable is primarily responsible for the difference in IR frequencies for hydrogen and deuterium?

6. The force constant for a CO molecule is 1860 N/m.

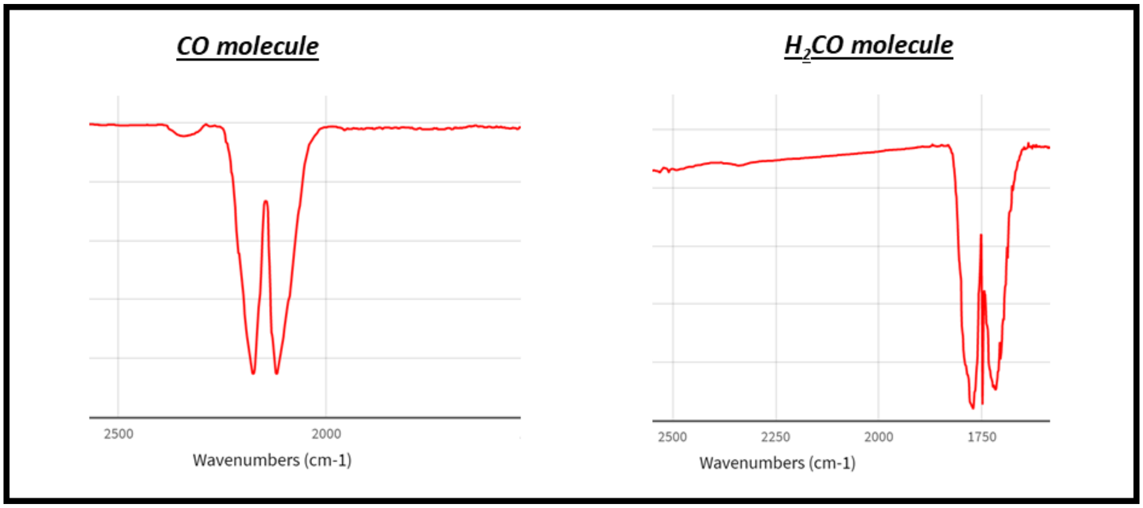
a) Calculate the zero-point energy for the CO molecule (in J/molecule). (Molar mass of carbon = 12.01 g/mol; molar mass of oxygen = 16.00 g/mol). REMEMBER UNITS!

b) How much energy (in J) is needed for a single CO molecule to move from the ground vibrational state to the first excited vibrational state?

c) What wavenumber does this correspond to? (This would be the peak position on an IR spectrum).

Problems

7. The figure below shows high-resolution IR spectra of the C-O vibrational peaks for a carbon monoxide molecule and a formaldehyde molecule (H_2CO). (Splitting of the peak is due to rotational transitions which will be addressed later in this course). As a first approximation, you can assume the reduced mass of CO and H_2CO are roughly the same. Use your knowledge of the harmonic oscillator model to explain why the C-O vibrational peaks are not at the same position. NO CALCULATIONS NEEDED!



Bonus Question: Use your understanding of the harmonic oscillator model and the provided spectrum to predict the ratio of force constants of H_2CO and CO.

Harmonic Oscillator Worksheet – KEY

Prior Knowledge:

These questions are to help you review information you have learned previously and will be helpful in this activity.

1. a) What is the mathematical relation between wavelength (λ) and frequency (υ)?

$$\lambda = \frac{c}{\upsilon}$$

   b) What are the units of each variable?

λ has units of m or nm.

υ has units of 1/s or Hz.

2. a) Describe in your own words how wavenumber relates to wavelength and frequency and provide an equation showing the relation. (Note that although chemists refer to IR "frequencies", these numbers are actually reported in units of *wavenumbers*).

Wavenumber is the inverse of wavelength.

$$\tilde{\upsilon} = \frac{1}{\lambda} = \frac{\upsilon}{c}$$

   b) What are the units for wavenumber ($\tilde{\upsilon}$)?

Units of wavenumber are cm^{-1}.

3) The Newton (N) is a derived unit composed of SI base units. Break down the Newton into its component units.

$$N = \frac{kg \cdot m}{s^2}$$

Goals:

- *To recognize that the quantum harmonic oscillator provides a model for the quantized vibrational energy of diatomic molecules*
  - *To recognize that wavelength, frequency, and wavenumber are all used as different representations of energy*
  - *To understand the influence of reduced mass on the magnitude of a vibrational frequency*
- *To articulate how the relation between force constant and frequency allows for the identification of molecules through infrared spectroscopy*
- *To use knowledge of vibrational energy levels to explain IR spectra*

Harmonic Oscillator Model

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \qquad E = \left(n + \frac{1}{2}\right)h\upsilon$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \qquad h = 6.626\ x\ 10^{-34}\ J \cdot s$$

Key Questions

1. What is the relation between reduced mass (μ) and frequency? Describe in your own words.

Reduced mass is inversely related to frequency. As reduced mass increases, the frequency decreases as the square root of the mass.

2. What is the relation between force constant (k) and frequency? Describe in your own words.

Force constant is directly proportional to frequency. As force constant increases, frequency increases as the square root of force constant.

3. A $C - N$ single bond, $C = N$ double bond, and $C \equiv N$ triple bond will have IR frequencies at roughly 1100 cm^{-1}, 1660 cm^{-1}, and 2220 cm^{-1}, respectively. Use your knowledge of the relation between frequency and force constant to match each force constant to its corresponding C-N bond. NO CALCULATION NECESSARY!

4. $C \equiv N$	D. $1047.6\ N/m$
5. $C = N$	E. $1873.7\ N/m$
6. $C - N$	F. $460.0\ N/m$

1 – B, 2 – A, 3 – C

Exercises

4. a) Calculate the reduced mass of a **single** hydrogen *molecule*. Include units in your answer. (molar mass of hydrogen = 1.008 g/mol). Report your answer in kilograms.

$$\mu = \frac{\left(1.008\frac{g}{mol}\right)\left(1.008\frac{g}{mol}\right)}{1.008\frac{g}{mol} + 1.008\ \frac{g}{mol}} = 0.504\frac{g}{mol} \times \frac{1\ mol}{6.02\ \times 10^{23}\ molecules} \times \frac{1\ kg}{1000\ g}$$

$$= 8.37\ \times 10^{-28} kg$$

b) Calculate the reduced mass of a **single** deuterium *molecule*. Include units in your answer. (molar mass of deuterium = 2.014 g/mol). Report your answer in kilograms.

$$\mu = \frac{(2.014\frac{g}{mol})(2.014\frac{g}{mol})}{2.014\frac{g}{mol} + 2.014\ \frac{g}{mol}} = 1.007\frac{g}{mol} \times \frac{1\ mol}{6.02\ \times 10^{23}\ molecules} \times \frac{1\ kg}{1000\ g}$$
$$= 1.67\ \times 10^{-27} kg$$

5. a) Compare the values you calculated for the reduced mass of the hydrogen and deuterium molecules. What do you notice?

The reduced mass of the deuterium molecule is about double that of the hydrogen molecule.

b) The IR frequencies of hydrogen and deuterium are 4159.5 cm^{-1} and 2990.3 cm^{-1}, respectively. Calculate the force constants for a hydrogen and deuterium molecule. Force constants should be reported in units of N/m.

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \to k = 4\pi^2\upsilon^2\mu$$

$$Hydrogen\ force\ constant:$$

$$\upsilon = c\tilde{\upsilon} = \left(3 \times \frac{10^8 m}{s}\right)\left(4159.5\frac{}{cm}\right)\left(\frac{100\ cm}{1m}\right) = 1.25 \times 10^{14} Hz$$

$$k = 4(3.14159)^2(1.25 \times 10^{14} Hz)^2(8.37 \times 10^{-28} kg) = 514.5\frac{kg}{s^2} = 514.5\ N/m$$

$$Deuterium\ force\ constant:$$

$$\upsilon = c\tilde{\upsilon} = \left(3 \times \frac{10^8 m}{s}\right)\left(2990.3\frac{}{cm}\right)\left(\frac{100\ cm}{1m}\right) = 8.97 \times 10^{13} Hz$$

$$k = 4(3.14159)^2(8.97 \times 10^{13} Hz)^2(1.67 \times 10^{-27} kg) = 530.6\frac{kg}{s^2} = 530.6\ N/m$$

c) Compare the values you calculated for the force constants of the hydrogen and deuterium molecules. What do you notice?

They are relatively close to each other in magnitude with deuterium being slightly larger than hydrogen.

d) Based on the harmonic oscillator model and your calculated values for reduced mass and force constants, what variable is primarily responsible for the difference in IR frequencies for hydrogen and deuterium?

Since there is a large difference between the IR frequencies, the force constants are fairly similar, and the reduced mass of deuterium is double that of hydrogen, it makes sense that the inverse relation of reduced mass and frequency would be primarily responsible for the difference in IR frequencies. When plugged into the harmonic oscillator model, the frequency of hydrogen would be larger than the frequency of deuterium. Since frequency and wavenumber (ie: IR frequency) are directly proportional to one another, the IR frequency of hydrogen would be larger than the IR frequency of deuterium as well.

6. The force constant for a CO molecule is 1860 N/m.

d) Calculate the zero-point energy for the CO molecule (in J/molecule). (Molar mass of carbon = 12.01 g/mol; molar mass of oxygen = 16.00 g/mol). REMEMBER UNITS!

$$\mu = \frac{(12.01\frac{g}{mol})(16.00\frac{g}{mol})}{12.01\frac{g}{mol} + 16.00\frac{g}{mol}} = 6.86\frac{g}{mol}\ x\ \frac{1\ kg}{1000\ g}\ x\ \frac{1\ mol}{6.02\ x\ 10^{23} molec}$$
$$= 1.14\ x\ 10^{-20}\ kg$$

$$v = \frac{1}{2\pi}\sqrt{\frac{1860\ N/m}{1.14\ x\ 10^{-20}\ kg}} = 6.43\ x\ 10^{13}\ Hz$$

$$Eo = \frac{1}{2}hv = \frac{1}{2}(6.626\ x\ 10^{-34} J \cdot s)(6.43\ x\ 10^{13} Hz) = 2.13\ x\ 10^{-20}\ J$$

e) How much energy (in J) is needed for a single CO molecule to move from the ground vibrational state to the first excited vibrational state?

$$Eo = \frac{1}{2}hv;\ E1 = \frac{3}{2}hv$$

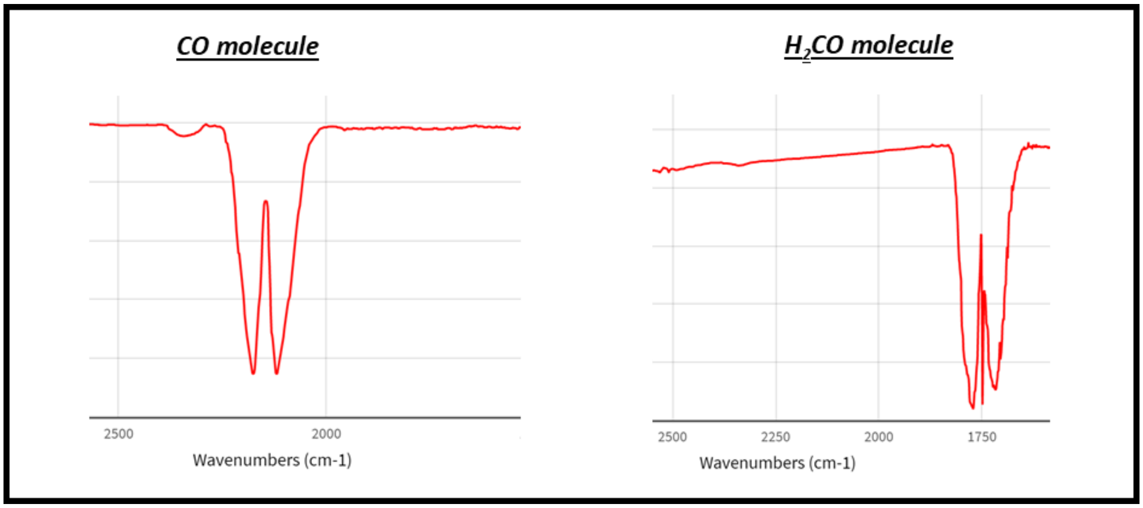
$$\Delta E = \frac{3}{2}hv - \frac{1}{2}hv = hv = (6.626\ x\ 10^{-34}\ J \cdot s)(6.43\ x\ 10^{13}\ Hz) = 4.26\ x\ 10^{-20}\ J$$

f) What wavenumber does this correspond to? (This would be the peak position on an IR spectrum).

$$\tilde{v} = \frac{v}{c} = \frac{6.43\ x\ 10^{13}\ Hz}{3\ x\ 10^{8}\ m/s} = \frac{214{,}333.33}{m}\ x\ \frac{1\ m}{100\ cm} = 2143.3\ cm^{-1}$$

Problems

7. The figure below shows high-resolution IR spectra of the C-O vibrational peaks for a carbon monoxide molecule and a formaldehyde molecule (H_2CO). (Splitting of the peak is due to rotational transitions which will be addressed later in this course). As a first approximation, you can assume the reduced mass of CO and H_2CO are roughly the same. Use your knowledge of the harmonic oscillator model to explain why the C-O vibrational peaks are not at the same position. NO CALCULATIONS NEEDED!



In the CO molecule, the C-O bond is a triple bond, and in the H_2CO molecule, the C-O bond is a double bond, meaning that the C-O triple bond is stiffer (higher force constant) than the C-O double bond. Since force constant is directly proportional (by the square root) to the frequency, the CO molecule should have a higher frequency (and IR frequency) than the H_2CO molecule (assuming reduced masses are approximately equal).

Bonus Question: Use your understanding of the harmonic oscillator model and the provided spectrum to predict the ratio of force constants of H_2CO and CO.

Taking the ratio of the peak positions from the spectra:

$$\frac{\upsilon(CO)}{\upsilon(H2CO)} \cong \frac{2150}{1750} = 1.23$$

And assuming k is approximately proportional to bond order:

$$\frac{\upsilon(CO)}{\upsilon(H2CO)} = \frac{\frac{1}{2\pi}\sqrt{\frac{k(CO)}{\mu}}}{\frac{1}{2\pi}\sqrt{\frac{k(H2CO)}{\mu}}} = \sqrt{\frac{k(CO)}{k(H2CO)}} \cong \sqrt{\frac{3\ bonds}{2\ bonds}} = 1.22$$

We can argue that the ratio of the peak positions is a good first approximation for the ratio of the force constants.