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The Curious Case of Concept: A Nation-Wide Survey of Faculty Beliefs About Quantum Mechanics Concept Inventories Uncovers New Details Regarding Physical Chemistry Experts' Understanding of Conceptual Knowledge.

Matt Smiley
Western Washington University, matthewbrandonsmiley@gmail.com

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By

Matthew B. Smiley

Accepted in Partial Completion

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ADVISORY COMMITTEE

Dr. Erin Duffy

Dr. Norda Stephenson

Dr. Tim Kowalczyk

GRADUATE SCHOOL

Dr. David L. Patrick, Dean

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Matthew. B. Smiley
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ABSTRACT. According to the chemistry education literature, physical chemistry educators strongly believe developing students' conceptual understanding is important[1]; however, the vast majority of educators (84%) were found to assess students predominantly on mathematical knowledge[2,3]. To better serve students of physical chemistry, the cause of misalignment between stated learning goals and assessment needs to be elucidated. To this end, the Faculty Perceptions of Published Quantum Mechanics Assessments Survey (FPPQMA) was developed. The FPPQMA is designed to probe physical chemistry educators' beliefs regarding the dichotomy between conceptual and mathematical knowledge[2]. In addition to free response questions that ask respondents to define conceptual and mathematical knowledge, the FPPQMA asks participants to categorize published quantum chemistry concept inventory questions[4-7] as "mostly mathematical, mostly conceptual, equally mathematical & conceptual, or other." The survey was designed with paired sets of questions. Each set of questions is best described by a singular American Chemistry Society concept heading[8] (e.g., Light and Matter Interactions, Particle-in-a-box model, Postulates of Quantum Mechanics, etc.). Each question within a set has a different representational form (e.g., textual, graphical, or symbolic). Data from our survey revealed the influence of question design on experts' application of conceptual and mathematical labels and elucidated their beliefs about the unidirectional relationship between these two knowledge domains. Our results indicate that the misalignment between learning goals and evaluation does not result from methodology, but from how experts distinguish conceptual and mathematical knowledge [1,2,9].

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GLOSSARY.

ACS-CPT – The American Chemistry Society's Committee on Professional Training Supplement. A document outlining common ideas and topics covered in undergraduate physical chemistry courses.

CONTENT VALIDITY – The extent to which a measure represents all facets of a given construct.

FACE VALIDITY - The extent to which a test is subjectively viewed as covering the concept it purports to measure.

FPPQMA – Faculty Perceptions of Published Quantum Mechanics Assessments Survey

PHENOMONOGRAPHIC THEORETICAL FRAMEWORK – A theoretical framework which posits that the world is experience differently by individuals. As such, a complete description of phenomena is the sum of all individual interpretations.[10]

RELIABILITY – The degree of consistency or dependability with which the instrument measures the attribute it is designed to measure.[11]

QPCS - Quantum Physics Conceptual Survey[7]

QCCI - Quantum Chemistry Concept Inventory[6]

QMCS - Quantum Mechanics Conceptual Survey[12]

QMCA - Quantum Mechanics Concept Assessment[4]

QMAT - Quantum Mechanics Assessment Tool[5]

QMFPS - Quantum, Mechanics Formalism and Postulate Survey[13]

QMVI - Quantum Mechanics Visualization Instrument[14]

QMS - Quantum Mechanics Survey[15]

TECHNOLOGICAL-SOCIAL DUALISM – A social theory positing that in scientific fields technical skills are values over social competence.[16]

VALIDITY - The degree to which an instrument measures what it is intended to measure.[17]

CHAPTER 1: CONCEPT

1.1: INTRODUCTION. The challenges of learning physical chemistry are many. Students must learn a complex network of terms, symbols, equations, formulae, processes, ideas, and concepts, and must be able to describe a host of new, increasingly abstract, chemical scenarios with ever more sophisticated mathematical tools[17,18]. In addition to the intellectual exercises required to learn physical chemistry, students must develop process and laboratory skills[19]. Students learn to work with new instrumentation and develop familiarity with in-depth laboratory procedures, often working with gasses and air free experimental setups. To put this all succinctly: learning physical chemistry is challenging for students. To complicate the matter further, there is disagreement among students and educators as to what challenges most hinder students' success in physical chemistry[20]. From the student perspective, physical chemistry is inherently challenging, abstract, math heavy, and students often enter physical chemistry classrooms believing themselves to have a low probability of success[1,20,21]. Educators believe that factors outside of their control inhibit student success. Factors like lack of time dedicated to teaching (due to other requirements such as research and committee work), minimal resources, and lacking professional development oppourtiunties[1,2]. Additionally - and most relevant to this study - educators commonly believe one of the primary obstacles to student success in physical chemistry is students' inability to make connections between the concepts pertinent to the discipline[2]. Contemporary education research tells us that meaningful learning in any discipline occurs as the result of students' ability to comprehend, connect, and synthesize many components inherent to a discipline; facts in isolation do little to better one's useful knowledge of a subject[22,23]. Because many educators believe students struggle to make connections between concepts, an emphasis on the development of conceptual understanding is common in curricula[1,2]. Despite the prevalence of conceptual understanding as a learning goal, assessment materials that focus on students' mathematical abilities are reported to be the norm in physical chemistry classrooms, nationwide[1-3]. Fox and Roehrig reported that the majority of assessment materials used by physical chemistry educators focused predominantly on mathematical reasoning, algorithmic processes, and quantitative problem-solving skills[1,3]. This manuscript study was born from a desire to find a rationale for this discrepancy, and began with what – naively - seemed a simple question: If educators wish for students to develop a conceptual understanding of physical chemistry, what are the concepts?

1.2: WHAT IS A CONCEPT?

To date, no formal definition of concept as it pertains to physical chemistry exists (zooming away from the lacking discipline specific definition, one finds that even from a philosophical perspective no singular characterization dominates the debate over what a concept truly *is*[24]). Colloquially, concepts are thought of as abstractions which occur in the mind[25]. Concepts are used to represent concrete objects, mental states, or abstract objects (and abstract ideas – like most ideas in quantum mechanics…) in generalizable ways[26]. The word concept is often used interchangeably with similar but distinct terms like idea, thought, notion, and theory. This manuscript does not intend to provide any justification for demarcation of these terms; Instead, each shall be considered synonymous and will be used to describe the mental tools that describe, categorize, and rationalize ideas pertinent to one's understanding of physical chemistry. After finding that the literature had little in the way of a working definition of concept within the domain of physical chemistry[9], we find it instructive to explore the ways in which physical chemistry educators *use* the term concept and attempt to identify what exactly the concepts of physical chemistry are assumed to be.

1.3: WHAT DO PHYSICAL CHEMISTRY EXPERTS THINK CONCEPTS ARE?

In the physical chemistry education literature, references to concept, conceptual learning, and conceptual education are ubiquitous[4,6,7,12]; however, no agreed upon formal definition exists which articulates precisely what these terms mean. The closest chemists have to a working definition of conceptual understanding comes from Holme et. al., in the general chemistry literature[27], who surveyed roughly 1400 chemists for their definitions of the term "conceptual understanding." Holme proposed a five-component definition articulating skills through which a student of chemistry might demonstrate conceptual understanding. As defined by Holme, a student could: *Transfer* core chemistry ideas to novel chemical scenarios, reason with *Depth* about chemistry ideas without relying solely on memorization, make *Predict[ions]* about chemical systems, *Problem Solve,* or *Translate* between scales and representations. We will return to Holmes' definition of conceptual understanding in section 1.4 but let us now turn our attention to the ways in which physical chemistry experts use a similar, possibly synonymous, term, "concept."

An analysis of topics identified by physical chemists in the relevant literature as "conceptual" revealed a lack of specificity as to what physical chemistry concepts actually are[5,13,15]. For example, in 2015, the American Chemical Society's Committee on Professional Training (ACS-CPT) published a Physical Chemistry Supplement[8] for educators which categorizes the term "quantum chemistry" as a "concept" and provides a list of common physical chemistry ideas, referred to as "terms", suggested to be subordinate to "quantum chemistry" by use of a heading-and-list format[26]. The list of terms includes items like "Postulates and Formations of Schrodinger Equations", "Operators and Matrices", "Particle-in-Box", and "Angular momentum"[8]. Throughout the literature, others topics are categorized as "concepts" by individual authors: "chemical bonding”[6], “orbitals”[28], “wave functions”[15], “angular momentum”[6], and “energy quantization”[14], to name only few, though none of these topics are identified as “concepts” by the ACS-PCT. Notice that the grain size for the term concept appears to be much larger when applied by the ACS-CPT (“quantum chemistry”), and smaller when applied by individual experts’ in their publications (“bonding”, “orbitals”, etc.). This may not constitute an actual problem. Quantum chemistry is a broad and diverse field, and it may be the case that the application of the term concept could vary between sub-disciplines[26]; however, it still remains troubling that so many educators desire their students to develop a skill (conceptual understanding) which relies largely on unagreed upon and undefined terms. More troubling still is the fact that a lacking formal definition of terms like concept, conceptual education, conceptual understanding, and conceptual learning has not hindered the development and publication of many instruments which proport to measure these entities in student populations.

1.4: HOW IS CONCEPTUAL UNDERSTANDING MEASURED?

Since the development of the Force Concept Inventory (a tool used to measure students’ understanding of forces in physics)[29], in 1992, concept inventories have been the gold standard for educators wishing to assess students’ domain specific knowledge[29]. Concept inventories are assessment instruments designed to evaluate specific skills, and/or knowledge, of students throughout a wide range of populations[6,29]. Generally, validation procedures for concept inventories (determining *what* a concept inventory measures) utilize iterative processes in which quantitative results from the inventory itself, and qualitative interviews with student populations and content experts in the field of applicability are used to determine the utility of a specific instrument[6,14,30,31]. Validated concept inventories often show very high reliability between student populations, varying academic institutions, and over many years of use[6], and thus are frequently used to quantify student learning gains[6]; however, concerns regarding the validity of these instruments exist[32]. Take for example an excerpt from the authors of the Quantum Mechanics Visualization Instrument (QMVI) – an instrument which purportedly measures students' conceptual understanding of quantum mechanical ideas by "focus[ing student's] attention on the core concepts [of quantum mechanics…by separating] them from the various levels of mathematical sophistication used to study them."[14]. The authors note, "the large jump in score for the QMVI over the course of the undergraduate career is perhaps a trick which, if students see once they typically recall."[14] In addition to concerns about what these tests actually measure, what a conceptual question *is* also remains undefined. Many educators appear to share the belief that conceptual questions are predominantly those without mathematical expression, and which often utilize a qualitative visual component, such as a diagram or picture, that represents the phenomenon in question[3,14, 28]. This loose definition leaves much to the imagination. Despite concerns regarding the validity of these instruments, and what about their design constitutes as conceptual, there remains a common belief among physical chemistry educators that concept inventories are capable of measuring students' conceptual understanding[7,31,32]. To date, eight published Quantum Mechanics concept inventories are available that claim to measure students' conceptual understanding over a range of topics commonly taught in physical chemistry[4-7,12-15]. A review of these studies found that almost no formal articulation was provided as to what aspects of instrument design (question content, question format, etc.?) constituted as conceptual. Further, the validation processes for most of these instruments rely predominantly on subjective expert opinion regarding the validity and reliability of the instrument[11,13]; but, as was found in our literature review of the application of the word concept, there is no expert consensus. Analysis of published concept inventories quickly yielded evidence of the possibility that these tools do not, in fact, measure what they proport to. Take for example, the Quantum Chemistry Concept Inventory (QCCI), which is a well-known, oft cited, concept inventory believed to be a very good measure of undergraduate physical chemistry students' conceptual knowledge[6]. Figure 1.1 shows item 10 in the QCCI. This item asks respondents to select the appropriate condition for a valid quantum mechanical wavefunction. This question could plausibly be answered using knowledge outside of the domain of chemistry (specifically, calculus) and known test taking strategies[34].

10. If a specific mathematical function is not ___ it can still be used as a wavefunction.
  a) antisymmetric
  b) continuous
  c) continuously differentiable
  d) integrable over all space

Figure 1.1: Question 10 From the Quantum Chemistry Concept Inventory. This figure shows question 10 from the well-known concept inventory, the QCCI. A student of introductory calculus (a prerequisite to physical chemistry) would be familiar terms like "continuous, continuously differentiable, and integrateable over all space." As such, one could use an elimination test taking strategy to select the correct answer, "antisymmetric", with no knowledge of the term antisymmetric itself.

If a question can be correctly answered without using knowledge of physical chemistry, is it not unreasonable to ask what does this question measure? It should be mentioned that the literature notes educators believe mathematical and conceptual knowledge are distinct domains (though intimately related)[1]. As such, it is entirely possible that the intended physical chemistry concepts being evaluated by question 10 of the QCCI are mathematical in nature. Let us return now to Holme's 5-component definition of conceptual understanding and use it as an analytical lens for analysis of the question shown in Figure 1. It appears that no one of the five components depicting a students' conceptual understanding, as proposed by Holme, shows any applicability to this inventory question. Students are not being asked to *Transfer* knowledge to a new domain nor reason about core ideas with *Depth* (more specifically, without memorization); they are not being asked to *Predict* anything about a chemical system, to *Problem Solve*, nor to *Translate* between representation or scale. Again, the Holme definition is found in the general chemistry literature, which could provide some rational for the lack of connection to the QCCI concept inventory question; however, it is the opinion of the authors of this thesis that some degree of generalizability between sub-disciplines of chemistry should be inherent in a definition of conceptual understanding, suggesting either that Holme's definition of conceptual understanding is incomplete, or that this QCCI question does not, in fact, measure conceptual understanding.

1.5: RESEARCH QUESTIONS/AIMS/FRAMEWORK. This study began by asking the seemingly simple question: what is a concept? As the study developed, it became clear that the scope of this question was simply too large for this, or likely any, singular study to determine (see Holme 2015 for a worthy attempt). Additionally, it may be the case that there is no practical reason to define what a concept formally *is,* as the appropriate definition may vary by discipline[26]. In lieu of a general, formal definition, it appears a useful exercise to determine *how* the term is being used by physical chemistry experts. This research was guided by the principals of phenomenography. Phenomenography, as a theoretical framework, assumes that individuals experience and interpret phenomena differently, as such, individual interpretations are considered incomplete. The complete description of a phenomenon is then the sum of all interpretations, as defined by each individual observer[10]. Further, this research was guided by three central research questions which arose during our preliminary investigation:

1) *How do physical chemistry experts view the nature of questions in QM concept inventories?*

2) *How do physical chemistry experts define conceptual vs. mathematical understanding?*

3) *What do physical chemistry experts view as the most important concepts and mathematical tools for students to learn in undergraduate QM?*

The research aims of the following manuscript are as follows:

1. *Elucidate physical chemistry educators' beliefs about the difference between conceptual and mathematical knowledge*[2].
2. *Contribute to the development of domain specific definition of the terms conceptual and mathematical knowledge*[1,9]
3. *Evaluate the impact surface-level features of question design (use of images, graphs, symbols etc.) have on physical chemistry educators' conceptualizations of assessment materials*[35].

CHAPTER 2: FACULTY PERCEPTIONS OF PUBLISHED QUANTUM MECHANICS ASSESSMENTS SURVEY

2.1: SURVEY DEVELOPMENT. The development process began with a literature review of published quantum chemistry and quantum physics concept inventories (many of the same principles are found in introductory classrooms of both these disciplines[36]). Using SciFinder, Google Scholar, and Web of Science, eight published concept inventories were identified: Quantum Physics Conceptual Survey (QPCS)[7], Quantum Chemistry Concept Inventory (QCCI)[6], Quantum Mechanics Conceptual Survey (QMCS)[12], Quantum Mechanics Concept Assessment (QMCA)[4], Quantum Mechanics Assessment Tool (QMAT)[5], Quantum, Mechanics Formalism and Postulate Survey (QMFPS)[13], Quantum Mechanics Visualization Instrument (QMVI)[14] , and the Quantum Mechanics Survey (QMS)[15]. As our study revolves around the definition and usage of the word concept, we determined only those surveys which self-identified as "conceptual" (i.e., used "conceptual" or "concept" in their title) would be included. Of the available inventories the following were selected: The QCCI[6], from the quantum chemistry literature; the QMCS[12] and the QMCA[4], from the quantum physics literature; and the QPCS[7] from the science education literature. An Excel document was created to organize the questions found in these concept inventories. This document included the concept inventory questions, the correct responses for each question, the type of representational form(s) used (symbolic, graphic, textual, or imaged based), and pairings with other questions of a different representational form but which map to the same ACS-APT topic[8]. From the eighty-six concept inventory questions found in the four concept inventories, twenty-four were selected for use in the FPPQMA. The selected questions met the following criteria:

- Have an even distribution of representational form – The final set of items in the FPPQMA needed to have similar amounts of textual questions, questions that include diagrams/images, and questions including symbolic nomenclature, such as mathematical formulae.

- Map to ACS-CPT's Physical Chemistry Supplement "topics list" – each item in the FPPQMA was required to map to a singular "topic" from the ACS-CPT's Physical Chemistry Supplement[8]; additionally, sets of items with varying representational forms needed to map to the same "topic" to parse out the effect of representational form while holding an items subject-matter constant.

- Be commonly taught subjects – each selected question needed to be a commonly taught subject, so it could be reasonably assumed that survey participants were familiar with the material[2].

Table 2.1 provides the final list of items selected for use in the FPPQMA, including the ACS topic and representational form best describing the item (complete questions are provided in the Supplementary Section). The selected questions were distributed throughout the survey in a way that minimized contiguation of representational form and ACS-CPT topic. The first iteration of the FPPQMA asked that respondents categorize each question with one of the following knowledge domain descriptions "Mostly Conceptual", "Mostly Mathematical", "Equally Conceptual and Mathematical", or "Other", following the prompt "To answer Assessment Item [X] successfully, what type of knowledge, if any, is required?". This prompt addressed research question 1, "how do physical chemistry instructors view the nature of questions in QM concept inventories?"

Table 2.1: Selected Survey Items for Use in the FPPQMA. This table shows the 20 items selected concept inventory questions which were used in the FPPQMA. The table shows the source of the question, the item number (found in the parent inventory), the ACS topic which describes the subject matter of the item, and the representational form of the item.

Source	Item #	Representational Form	ACS Topic	Pairing
QPCS	2	graph	Light-matter interaction	QPCS 2, QPCS 3
QMCS	1	image	Electronic spectra of atoms and molecules	QMCS 1, QMCS 3,
QPCS	20	text	Operators and matrix elements	QPCS 20, QPCS 21,
QMCS	11	graph, symbol	Postulates and formulations of Schrodinger equations	QCCI 7, QMCS 11
QCCI	5	text	Simple harmonic oscillator	QCCI 8, QCCI 5
QPCS	14	image, symbol	Wave-particle duality	QPCS 14 QPCS 8 QMCS 5
QMCA	10	graph, symbol	Particle-in-a-box	QMCS 6, QCCI 14, QMCA 10,
QMCA	34	text	Operators and matrix elements	QMCA 24, QMCA 34, QMCA 35
QMCS	3	image, symbol	Electronic spectra of atoms and molecules	QMCS 1, QMCS 3,
QPCS	3	text	Light-matter interaction	QPCS 2, QPCS 3
QPCS	8	text	Wave-particle duality	QPCS 14 QPCS 8 QMCS 5
QMCS	6	graph, symbol	Particle-in-a-box	QMCS 6, QCCI 14, QMCA 10,
QCCI	7	text	Postulates and formulation of Schrodinger equations	QCCI 7, QMCS 11
QCCI	14	text	Particle-in-a-box	QMCS 6, QCCI 14, QMCA 10,
QCCI	12	Symbol	Postulates and formulations of Schrodinger equations	-
QMCA	35	symbol	Operators and matrix elements	QMCA 24, QMCA 34, QMCA 35
QCCI	8	text	Vibrational spectra	QCCI 8, QCCI 5
QMCS	5	symbol	Wave-particle duality	QPCS 14 QPCS 8 QMCS 5
QPCS	21	text	Operators and matrix elements	QPCS 20, QPCS 21,
QMCA	24	symbol	Spin	QMCA 24, QMCA 34, QMCA 35

Participants were subsequently asked "What specific conceptual and/or mathematical knowledge, if any, is required to answer Assessment Item [X] successfully?" and asked to provide a list (up to 10) of concepts relevant to the question. This prompt addressed research question 3, "What do physical chemistry instructor's view as the most important concepts and mathematical tools for students to learn in undergraduate QM?".

A question explicitly targeting the relationship between representational form and how participants categorized the knowledge domain best describing the question was included. "What features (e.g., content, format, visual components) of Assessment Item [X] led to your choice [in categorizing the type of knowledge]?" This question was intended to encourage participants of the survey to describe what features of the survey items lead to their knowledge domain assignments. Last, participants were asked "For what course level in chemistry, if any, is Assessment Item [X] appropriate?" with response options: "Undergraduate Chemistry", "Undergraduate physical chemistry", "Graduate-level chemistry" and "Other (please specify)". When our group members (principal investigator, Dr. Erin Duffy, primary author and graduate researcher, Matt Smiley, and undergraduate researcher, Tiffany Chamberlain) performed time trials on this survey draft, operating under the assumption that participants would answer all survey questions, it was determined that the duration of the survey would be too long to anticipate an acceptable return rate (X = 34.00 min, n = 3). After careful consideration, the number of questions was reduced to twenty. The four questions removed were chosen due to their similarity to others which would remain in the survey. The duration of the survey was still too long after this abridgement, and it was determined that participants would receive a five-question subset of the full survey, instead of interacting with all 20 items. This end was achieved using Qualtrics Behavior Functions. The behavior functions are capable of randomizing question delivery and ensuring an equal proportion of each question is administered to the participant pool.

The questions targeting the appropriate course level for the survey item were removed, as they did not align clearly with our proposed research questions. Additionally, each participant of the survey would be requested to provide demographic information including the most recent time they taught a physical chemistry course, the number of years they have been teaching physical chemistry, and the nature of their own research (binned as "Experimental", "Theoretical/Computational", "physical chemistry Education", and "Does not conduct research in physical chemistry."). These data points would be later used to determine if there was any correlation between experience/expertise and the way physical chemistry experts categorized physical chemistry concept inventory materials. Participants were also asked if they consented to a follow-up interview should the researchers on this project determine the need.

The initial draft of the FPPQMA concluded with four open-ended prompts reading:

1. "In your own words, what is a conceptual understanding?"
2. "In your own words, what is a mathematical understanding?"
3. "What are the most important concepts (up to 10), if any, for students to take away from an undergraduate physical chemistry course focused on quantum mechanics?"
4. "What are the most important mathematical tools (up to 10), if any, for students to take away from an undergraduate physical chemistry course focused on quantum mechanics?"

These concluding prompts were provided to each participant, regardless of what subset of the concept inventory questions they received. At this point in the development of the FPPQMA, our group reached out to Dr. Jack Barbara of Portland State University. Dr. Barbara is an expert in the design and implementation of qualitative surveys, in the realm of chemistry education[37]. Dr.

Barbara's guidance led us to move prompts 1 and 2 to the beginning of the survey, as it was believed that the participant responses would be more general if asked these questions before being influenced by the content of the survey itself. The threshold of 10 items on prompts 3 and 4 was lowered to 5 items because we believed that allowing a larger threshold would invite more general responses. Last, the free response component "What specific conceptual and/or mathematical knowledge, if any, is required to answer Assessment Item [X] successfully?" was integrated, as a text box, associated with the respondent's knowledge domain selection ("Mostly Conceptual", "Mostly Mathematical", etc.) to ensure clear associations between the selected knowledge domain and the concepts provided by the participant. Responses from a pilot survey (See 2.2 Survey Validation) made it clear that our question asking "what features [of a concept inventory question led to a respondent's categorization]" was confusing to participants. Most replies to this question were simply the word "content" in lieu of a description of *what* content, or more specifically, what *about* the content had influenced their response (as we had envisioned). This question was ultimately removed. For the final draft of the FPPQMA survey we decided to include two questions we believed would help us better understand not only what physical chemistry experts believed about the concept inventory questions, but what they believed about their *students'* interactions with these materials. These prompts were inspired by the *Depth* component of Holme's 5-component definition of conceptual understanding[9]. We decided on the following questions:

1) To what extent does a student need to understand the concept(s)/mathematical tool(s) you mentioned above to know which is the correct answer choice?

2) To what extent does a student need to understand the concept(s)/mathematical tool(s) you mentioned above to be able to explain why the answer choice is correct?

Each of the two questions had the following radio button options associated with them:

- They must have a deep understanding of the concept(s)/mathematical tool(s) to determine the correct choice.
- They can have only a superficial understanding of the concept(s)/mathematical tool(s) and rote memorization of facts/algorithms to determine the correct choice.
- They can rely only on rote memorization of facts/algorithms to determine the correct choice.

Time trials were again performed by our group members, and it was determined that the survey should take respondents approximately 10-15 minutes to complete. This was deemed an acceptable length. All items on the final FFPQMA survey can be found in the supplemental section of this thesis.

2.2: SURVEY VALIDATION. The validation process for the FPPQMA consisted, in part, of regular group discussion between the principal investigator of this thesis, Dr. Erin Duffy, the primary author and graduate researcher, Matt Smiley, and an undergraduate researcher, Tiffany Chamberlain, through which all materials appropriate to our stated project goals and research questions were selected. As the survey is composed from previously published physical chemistry concept inventories, content-validity was never in question; however, as the survey was designed to probe not only physical chemistry educators' beliefs about materials from published inventories, in a general sense, but also to determine if superficial features of the questions, themselves, could influence an educators' beliefs about the material, face-validity was of concern.

This was one of the reasons for the removal of an aforementioned draft question that attempted to directly probe the influence that surface features of inventory questions have on expert responses. As part of the validation process, the survey was assessed by Dr. Jack Barbara, of Portland State University – an expert on qualitative survey design and administration[37]. Through Dr. Barbara's guidance and the survey's prompts were streamlined and vetted to best meet desired outcomes, in alignment with our research questions.

2.3: SURVEY PILOT & ADMINISTRATION. To ensure our sample population was as wide reaching and comprehensive as possible, we turned to the American Chemistry Society for a list of all institutions within the United States that have ACS-approved chemistry programs. The ACS-approved chemistry program list held 688 institutions, each categorized by state, ACS region, Carnegie Classification, and highest degree offered by the institution. For each institution on the ACS-approved program list, a university website was located using Google, and, by sheer force of will, the members of our group painstakingly mined each website for faculty contacts. Faculty selected for this study were those who were identified as physical, theoretical, or computational chemists. Determinations of these specializations were based on departmental categorizations (e.g., as physical, theoretical, or computational chemists) of their faculty. Once a faculty member was determined to be a physical, theoretical, and/or computational chemist, their name and contact were input into an Excel document used to organize participant information. The list of suitable participants for the FPPQMA totaled 1918 individuals. A pilot study consisting of 104 individuals selected from a range of institutions (both geographical and Carnegie classification) was undertook. These universities used in the pilot study of the FPPQMA are listed in Table 2.2.

Table 2.2: List of Participants involved in Pilot Study. This table shows the universities involved in the FPPQMA Survey pilot study, and details regarding their categorization.

Name	ACS Region	US Region	State	Highest Chem Degree
Alma College	Great Lakes	Midwest	MI	Bachelor's
Cedar Crest College	Mid-East	Northeast	PA	Bachelor's
Duke University	Southeast	Southeast	NC	Ph.D.
Humboldt State University	Far West	West	CA	Bachelor's
Johns Hopkins University	Mid-East	Northeast	MD	Ph.D.
Kalamazoo College	Great Lakes	Midwest	MI	Bachelor's
Lamar University	Southwest	Southwest	TX	Master's
Loyola University New Orleans	Southeast	Southeast	LA	Bachelor's
Montana State University	Rocky Mountains	West	MT	Ph.D.
New Mexico Highlands University	Southwest	Southwest	NM	Master's
New Mexico State University Main Campus	Southwest	Southwest	NM	Ph.D.
Reed College	Far West	West	OR	Bachelor's
Southwestern University	Southwest	Southwest	TX	Bachelor's
Syracuse University	Mid-East	Northeast	NY	Ph.D.
University of Arizona	Southwest	Southwest	AZ	Ph.D.
University of California-Riverside	Far West	West	CA	Ph.D.
University of Mary Washington	Southeast	Southeast	VA	Bachelor's
University of Minnesota-Morris	Plains	Midwest	MN	Bachelor's
University of Missouri - Saint Louis	Plains	Midwest	MO	Ph.D.
University of North Dakota	Plains	Midwest	ND	Ph.D.
University of Richmond	Southeast	Southeast	VA	Bachelor's
Utica College	Mid-East	Northeast	NY	Bachelor's
Virginia Polytechnic Institute and State University	Southeast	Southeast	VA	Ph.D.
Wellesley College	New England	Northeast	MA	Bachelor's
Willamette University	Far West	West	OR	Bachelor's

The pilot study received a return rate of 7.7 % (n=8), which was slightly below the 10% expected from similar studies[9]. Following adjustments to the survey (noted in 2.1 Survey Development) and abiding by the communication regulations of Western Washington University, and those established by the Institutional Review Board for this research project, the 1918 potential participants of our study received a brief email From Dr. Duffy, shown in Figure 2.1, inviting them to participate in our survey. After one week, participants who had not replied were sent an email reminder inviting them to participate. The data collection period of the survey was a duration of 14 days.

Dear Prof. <Last Name>,

My name is Erin Duffy, and I am an Assistant Professor of Chemistry at Western Washington University in Bellingham, WA. I am inviting you to participate in a survey because you are listed as a physical, theoretical, and/or computational chemist on your department website. This survey is designed to investigate faculty beliefs about conceptual and mathematical learning in undergraduate quantum mechanics courses. The survey should take approximately 10-15 minutes to complete. If you are willing to participate in this study, please follow the link to the survey below:

Survey Link: <Survey Link Here>

If you have any questions or concerns, please feel free to contact me at duffye@wwu.edu.

Thank you for your time,
Erin

--
Erin M. Duffy, PhD
Assistant Professor, Department of Chemistry and
Science, Math, and Technology Education (SMATE)

Western Washington University
Department of Chemistry
516 High St – MS 9150
Bellingham, WA 98225

Figure 2.1: Survey Invitation Letter from Dr. Duffy to Potential Participants of the FPPQMA. This figure shows the generic form of the invitation letter from Dr. Duffy to potential participants of the FPPQMA Survey. The Letter depicts what we are intending to study, why a participant was selected for the study, and the expected duration for completion.

CHAPTER 3. DATA AND RESULTS

3.1: CODEBOOK. A portion of the data obtained from the administration of the FPPQMA was in the form of written free responses to the questions, “In your own words, what is a conceptual understanding?” and “In your own words, what is a mathematical understanding.” To decipher this data, a coding scheme was developed. The development of a coding scheme is an iterative process through which researchers create a list of words or short phrases (codes) that catalogue the prevalence of ideas pertaining to their research questions[38]**.** The proper application of codes allows researchers to “signal what is going on in a piece of data in a way that links it to some more general issue.”[38]. To develop our coding scheme, we began by having each group member “open-code” a subset of the data. The objective of open coding is to begin noticing trends and themes and to determine preliminary descriptions of these themes. Figure 3.1 shows a sample portion of Dr. Duffy’s preliminary code structure. In Figure 3.1, notice that descriptions of individual events like “[one’s] ability to read graphs” are nestled under headings which position these events into larger themes (in the case of ““[one’s] ability to read graphs”, the heading theme is “Demonstrate Understanding.”). Following preliminary open coding, our group held many discussions of the emergent patterns, themes, and made proposals for structural organization. As expected from results found in a similar study[9], our data reflected that participants hold a wide range of definitions and beliefs about the nature of conceptual and mathematical knowledge. Many of the definitions provided were from the perspective of how students could possess and/or demonstrate their understanding of conceptual and mathematical knowledge in physical chemistry, instead of what these terms mean outside of the range of academia. This was reasonable considering the context of the FPPQMA, which uses evaluation

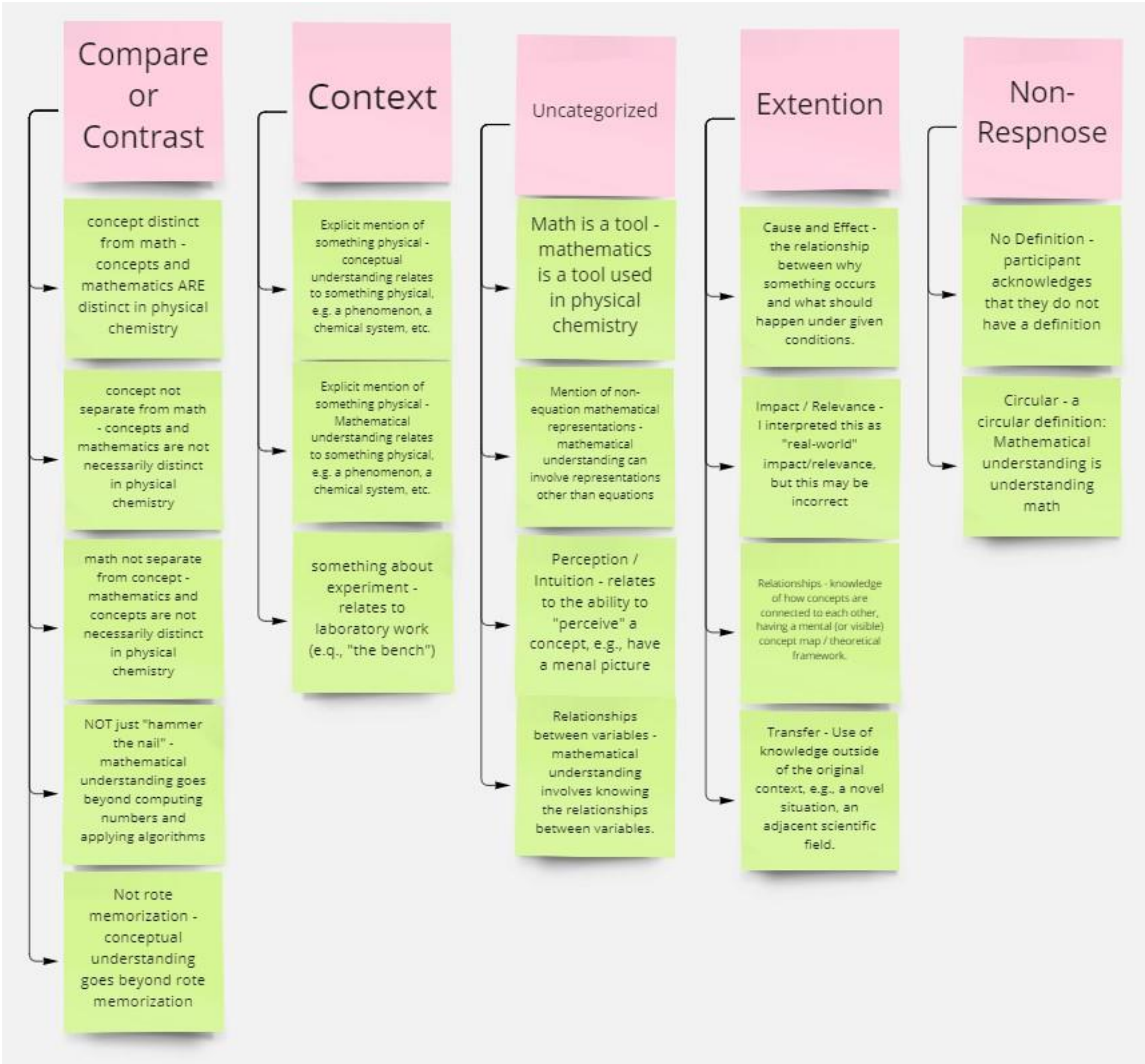

Figure 3.1: Sample portion of Dr. Duffy's Preliminary Coding Scheme. This figure shows Dr. Duffy's first draft of a coding scheme, in the software Miro, used to describe themes found in the FPPQMA survey data. The general structure of this coding scheme includes response categories (shown in pink) which themselves encompass subsets of more specific participant responses (shown in green).

materials from published concept inventories; participants are primed to think about these questions from a pedagogical perspective. Participant responses ranged from various forms of communication one might use (verbal, written, or symbolic) to convey their conceptual or mathematical understanding, to more ephemeral notions that demonstrate understanding, like how various subjects and discipline connect, how theory applies to novel situations, and examples of the mathematical tools and functions necessary for a grasp of physical chemistry. Each group member's individual coding scheme was transcribed into a collaborative whiteboard using the visualization software Miro. Within Miro, codes proposed by group members were grouped according to similarity, and through multiple discussions the individual codes were merged to form the complete list of codes used in our study. Figures 3.2 and 3.3 show the Miro White Board used to organize our coding scheme. The coding scheme used to analyze the FPPQMA data is broken into four general categories: Conveying understanding, Context of Physical Phenomena, Epistemological, and Other. Each category includes multiple sub-categories (the codes themselves), which were developed through a combination of literature grounded precedent[9], and emergence via observation. A Complete list of codes in our coding scheme and their respective definitions is provided in Table 3.1.

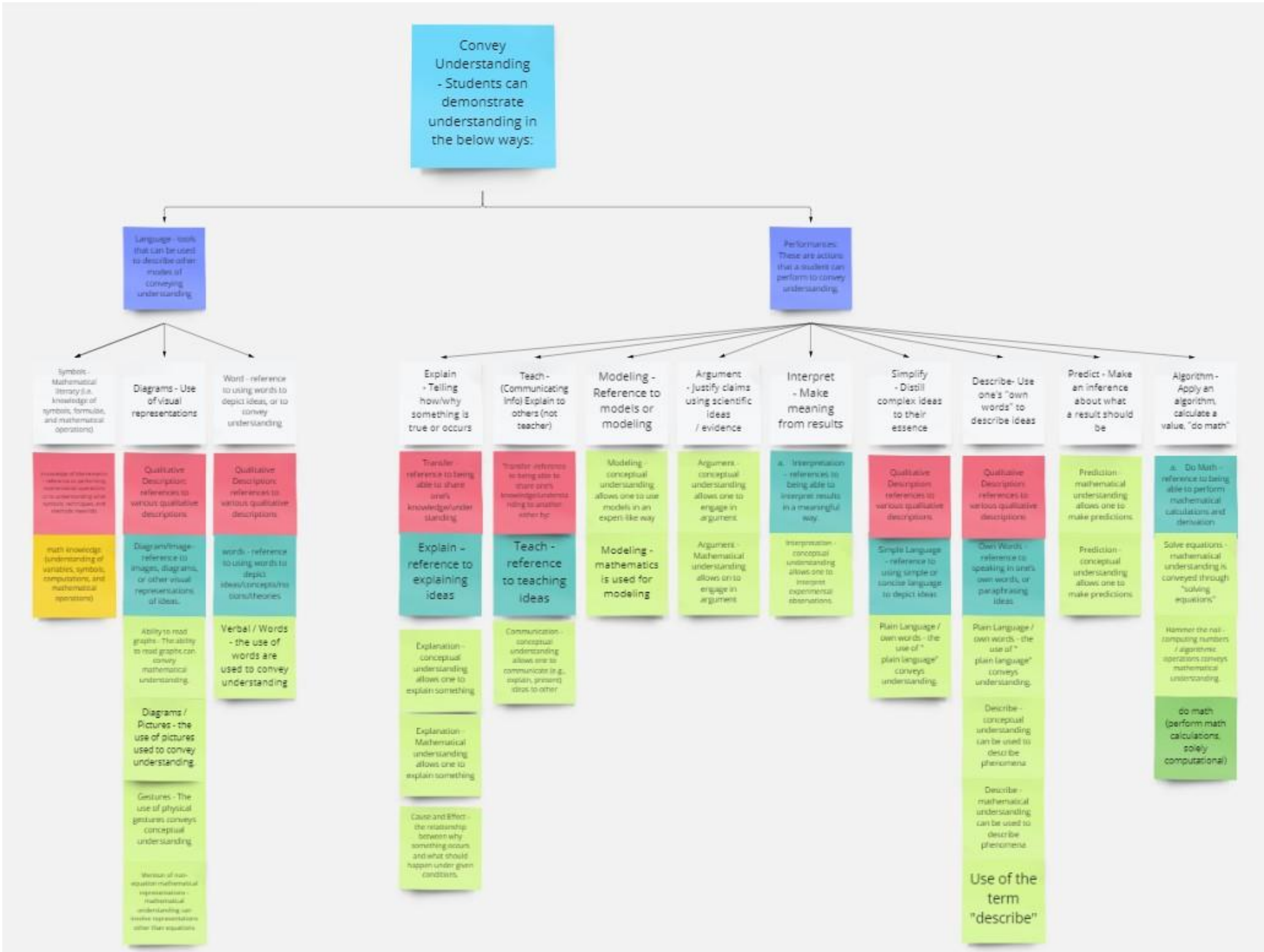

Figure 3.2: Coding Scheme Developed for the FPPQMA (Part 1). This figure depicts the coding scheme developed to describe the qualitative data collected from the FPPQMA survey. The largest blue boxes are the 4 primary categories. Sub-categories are broken into two tiers: purple is a sub-heading, and white boxes depict the codes themselves. Below the codes (white) are notes that describe the criteria for the application of each code.

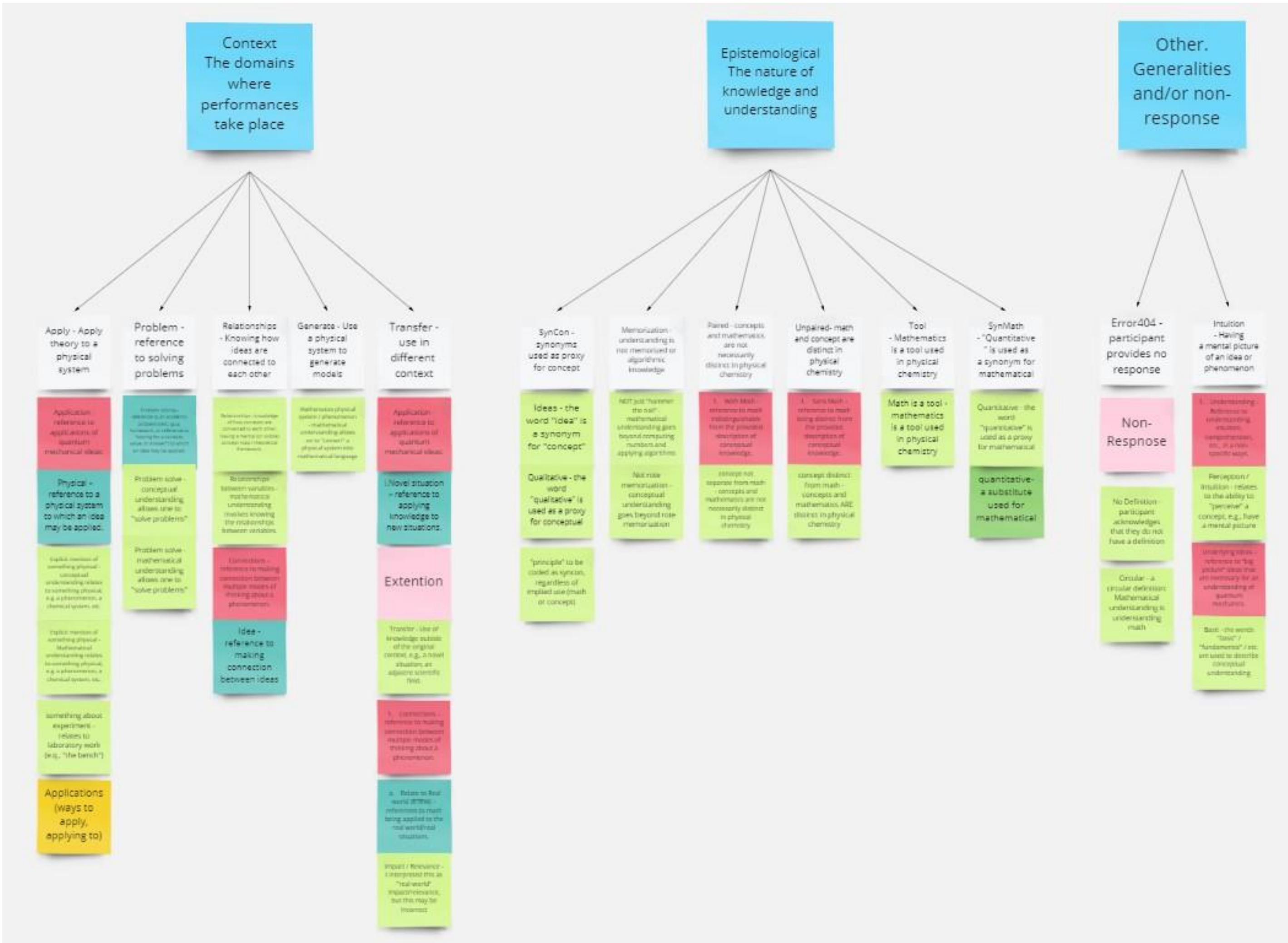

Figure 3.3: Coding Scheme Developed for the FPPQMA (Part 2). This figure depicts the coding scheme developed to describe the qualitative data collected from the FPPQMA survey. The largest blue boxes are the 4 primary categories. Sub-categories are broken into two tiers: purple is a sub-heading, and white boxes depict the codes themselves. Below the codes (white) are notes that describe the criteria for the application of each code.

Table 3.1: List of Codes Developed for Qualitative Analysis of FPPQMA Survey Data.

Language - Tools that can be used to describe other modes of conveying understanding			
Symbols	Reference to mathematical literacy (e.g., knowledge of symbols, formulae, and mathematical operations), or mention of mathematical components (e.g., variables, equations, techniques, etc.), operations, or symbols.	*Diagrams*	Reference to images, diagrams, graphs, pictures, and non-equation/non-verbal mathematical representations.
Word	Reference to using written or spoken words to depict ideas and/or to convey understanding.		
Performances - These are actions that a student can perform to convey understanding			
Explain	References to demonstrating one's knowledge and/or understanding by telling how/why something is true or occurs, which may include describing "cause and effect", using mathematical tools, or non-specific use of the word "explain".	*Algorithm*	References to being able to perform, solve, or compute mathematical calculations, operations, and derivation.
Teach	Reference to being able to share/communicate one's knowledge with another (not teacher).	*Describe*	Reference to using one's "own words" to describe ideas.
Modeling	Reference to models or modeling, using models in an expert-like way, and/or to mathematics being used for modeling.	*Simplify*	Reference to distillation of complex ideas to their essence, e.g., using simple, plain, or concise language to depict ideas. (Note: non-specific references to "basic" or "fundamental" concepts are coded as intuition).
Argument	Reference to the justification of claims using scientific ideas and/or evidence to another.	*Predict*	References to making an inference about what a result should be.
Interpret	References to being able to make meaning from results and/or data.		
Context - The Domains where performances take place			
Relationships	References to relationships between physical chemistry tools (models/math) and their applications, different modes of thinking (e.g., connection between different knowledge domains), or variables in an equation; knowing how concepts are connected to each other; having a mental (or visible) concept map / theoretical framework.	*Generate*	References to the generation of a model (e.g., mathematizing a physical system) based on observation or knowledge of the system.
Apply	References to the application of a concept, theory, or idea, to a physical system. Physical systems include references to chemical systems, experiments, and synonyms like phenomenon and observation. (Note: the verbs "explain" and "describe" are not example of apply).	*Transfer*	References to use of quantum mechanical ideas in a new context, adjacent scientific field, or the "real world" (e.g., climate change, industrial applications, etc.)
Epistemological – The nature of knowledge and understanding			
Unpaired	References to conceptual knowledge and mathematical knowledge being distinct domains in physical chemistry.	*SynMath*	Use of "quantitative" as a synonym for mathematical.
Memorization	Reference to understanding not being memorized or algorithmic.	*Tool*	Reference to mathematics being a tool used to perform functions related to physical chemistry.
SynCon	synonyms for concept, including "idea", "qualitative", and "principle".		
Paired	References to conceptual knowledge and mathematical knowledge not necessarily being distinct domains in physical chemistry.		
Other – Generalities and/or non-response			
Intuition	References to understanding, intuition, perception or comprehension of ideas, concepts, or tools necessary for physical chemistry in non-specific ways. Unspecific uses of the words "basic" and "fundamental" are to be coded as intuition.	*Error404*	Respondent stated they chose not to answer the question, acknowledged they had no definition, provided a circular response, or a response which did not correlate to the question prompt.

3.2: INTER-RATER RELIABILITY. Following the development of our coding scheme, the need to determine how reliably each of our coders was applying the scheme to our data was a necessity. The metric determined most suitable for this task was the Fleiss Kappa Inter-Rater Agreement Index. Fleiss Kappa is a quantitate index used to compare how consistently multiple independent raters apply the same qualitative judgments to categorical data sets[39-42]. Fleiss Kappa calculations rely on the ratio between observed rater agreement and that expected purely by chance (see the Supplemental Section S.3 for more on Fleiss Kappa). The result of Fleiss Kappa calculations is a value ranging from 0 to 1 (0 indicating no calculated agreement above that expected by chance, and 1 indicating perfect agreement)[40]. Fleiss Kappa calculations were performed on the codes our group applied to a forty-respondent sub-set of our data before coding the entire data set. This task was performed using Microsoft Excel and a statistical software called IBM SPSS Statistics. To complete this task, each code applied to the first forty respondents' provided definitions of Conceptual and Mathematical knowledge was tabulated and converted to binary using Excel's "COUNTIF" function, using the names of each individual code as search queries. Table 3.2 shows the tabulated codes in binary form. In the Table 3.2, a value of "1" indicates the code corresponding to the row heading has been applied by the coder named in the column heading (M = Matt, E = Erin, T = Tiffany), and a value of "0" indicates the corresponding code was not applied by the corresponding rater. These binary tabulations were sorted into individual sets, each representing the application of a specific code (i.e., "Teach", "Explain", "Paraphrase", etc.) to the forty participants. Table 3.3 shows our application of the code "Symbols" to the first 40 participants in our data. Using IBM SPSS statistics, the Fleiss Kappa values for each code in the IRR set were calculated. This process allowed us to parse out codes which needed more clarification, and those for which a reasonable assumption could be made that application from coder-to-coder would be consistent. Table 3.4 shows the Fleiss Kappa calculation results. Based on literature precedent, kappa values below a threshold of 0.60 were considered to have unacceptable agreement for our study[43]. For those codes below the 0.60 kappa threshold, group dialogues were held for the duration of the coding process to ensure these codes were applied consistently amongst group members.

Table 3.2: Tabulated Participant Data Converted to Binary. This table shows tabulated codes applied by our three independent coders to individual participants' responses. The binary conversion was performed by surveying the tabulated codes using Excel’s ”COUNTIF” function with individual codes names as search queries. The first letters represent the coder (M = Matt, E = Erin, T = Tiffany). The second letters indicate the prompt (C = Conceptual prompt. M = Mathematical prompt).

codes	1-CM	1-CE	1-C T	1-MM	1-ME	1-MT	2-CM	2-CE	2-C T	2-MM	2-ME	2-MT
Symbols	0	0	0	1	1	1	0	0	0	1	1	1
Diagram	0	0	0	0	0	0	0	0	0	0	0	0
Word	0	0	0	0	0	0	0	0	0	0	0	0
Explain	0	0	0	0	0	0	0	0	0	0	0	0
Teach	0	0	0	0	0	0	0	0	0	0	0	0
Modeling	0	0	0	0	1	0	0	0	0	0	1	0
Argument	0	0	0	0	0	0	0	0	0	1	0	0
Interpret	0	0	0	0	0	0	0	0	0	0	0	0
Problem	0	0	0	0	0	0	0	0	0	0	0	0
Simplify	0	0	0	0	0	0	0	0	0	0	0	0
Describe	0	0	0	0	0	0	0	0	0	0	0	0
Predict	0	0	0	0	0	0	0	0	0	0	0	0
Algorithm	0	0	0	0	1	1	0	0	0	1	1	1
Relationships	0	1	1	0	0	0	0	1	0	0	1	1
Intuition	1	1	1	0	0	0	1	1	1	1	0	1
Apply	0	1	0	0	0	0	0	0	0	0	0	0
Generate	0	0	0	0	1	0	0	0	0	0	0	0
Transfer	0	0	0	0	0	0	0	0	0	0	0	0
Transfer	0	0	0	0	0	0	0	0	0	0	0	0
SynCon	0	0	0	0	0	0	0	0	0	0	0	0
Memorization	0	0	0	0	0	0	0	0	0	0	0	0
Paired	0	0	0	0	0	0	0	0	0	0	0	0
Unpaired	0	0	0	1	1	1	1	1	1	0	0	0
Tool	0	0	0	0	0	0	1	0	0	0	0	0
SynMath	0	0	0	0	0	0	0	0	0	0	0	0
Error404	0	0	0	0	0	0	0	0	0	0	0	0

Table 3.3: Binary Data for the Code "Symbols". This table shows a binary tabulation of the code "Symbols" as applied by three independent coders (M = Matt, E = Erin, T = Tiffany) to the 40 participants used to determine our Interrater reliability. The second letters indicate the prompt (C = Conceptual prompt. M = Mathematical prompt).

Participant	CM	CE	CT	MM	ME	MT	Participant	CM	CE	CT	MM	ME	MT
1	0	0	0	1	1	1	*21*	0	0	0	1	1	1
2	0	0	0	1	1	1	*22*	0	0	0	1	0	1
3	0	0	0	1	1	1	*23*	0	0	0	0	0	0
4	0	0	0	0	0	0	*24*	1	1	1	1	1	1
5	0	0	0	0	0	0	*25*	0	0	0	1	1	1
6	1	1	1	1	1	1	*26*	0	0	0	0	0	0
7	0	0	0	1	1	1	*27*	0	0	0	1	0	1
8	0	0	0	1	1	1	*28*	0	0	0	0	1	1
9	0	0	0	0	0	0	*29*	0	0	0	0	1	1
10	0	0	0	0	0	0	*30*	0	0	0	1	1	1
11	0	0	0	1	1	1	*31*	1	0	0	1	1	1
12	0	0	0	0	0	0	*32*	0	0	0	0	0	0
13	0	0	0	1	1	1	*33*	0	0	0	0	0	0
14	0	0	0	0	0	0	*34*	0	0	0	1	1	1
15	0	0	0	0	0	0	*35*	0	0	0	1	1	1
16	0	0	0	1	1	1	*36*	0	0	0	0	0	0
17	0	0	0	1	1	1	*37*	0	0	0	1	1	1
18	0	0	0	0	0	0	*38*	0	0	0	0	0	0
19	0	0	0	0	0	0	*39*	0	0	0	0	0	1
20	0	0	0	0	0	0	*40*	0	0	0	0	0	0

Table 3.4: Tabulation of Fleiss Kappa Values by Code. This table shows Fleiss Kappa (*k)* calculations performed for each individual code as applied by our raters to a 40-participant sub-set of our data. Values below a literature grounded threshold[43] of $K = 0.6$ are shown in red.

Code Name	*K*	Code Name	*K*
Symbols	0.818	*Relationships*	0.591
Diagram	0.960	*Intuition*	0.640
Word	0.945	*Apply*	0.435
Explain	0.869	*Generate*	0.469
Teach	1.000	*Transfer*	0.829
Modeling	0.519	*SynCon*	0.666
Argument	0.561	*Memorization*	0.871
Interpret	0.573	*Paired*	0.304
Problem	0.799	*Unpaired*	0.636
Simplify	0.853	*Tool*	0.687
Paraphrase	1.000	*SynMath*	0.919
Predict	0.837	*Error404*	0.853
Algorithm	0.714	-	-

3.3: QUALITATIVE DATA. Qualitative data from the FPPQMA survey was comprised of applications of codes from our codebook (section 3.1: Codebook) to participant responses to the survey questions "In your own words, what is a conceptual understanding?" and "In your own words, what is a mathematical understanding?" These data were recorded and processed using Microsoft Excel. Table 3.5 shows a sample of these data in textual form. Each row in Table 3.5 corresponds to the codes applied to an individual participant's survey response. The titles "C" and "M" indicate the "Conceptual" and "Mathematical" prompts, respectively. Using Excel's "COUNTIF" function with the name of individual codes as search queries, the total instances of each code were calculated. These totals were divided by the net number of codes applied (n=1221) yielding the percentages of application reported in Table 3.6. Graphical representations of these percentages are provided in Figure 3.4 and a normalized distribution is shown in Figure 3.5. What is immediately apparent from Table 3.6 and Figure 3.4 is that the codes Intuition and Symbols were the two most frequently applied codes. The normalized data in Figure 3.5 indicated that Intuition was applied predominantly to the Conceptual prompt, while Symbols was applied predominantly to the Mathematical prompt. The codes Intuition, SynCon, Explain, Transfer, Unpaired, Diagram, Word, Describe, Simplify, Teach, Argument and Memorization were applied more frequently in response to the conceptual prompt (>55%), while the codes Symbols, Algorithm, SynMath, Problem, Tool, Interpret, Generate, Paired and Modeling were applied more frequently to the mathematical prompt (>55%).

Table 3.5: List of Codes Applied to Participant Responses. This table shows a sample of codes applied to participant responses to the prompts, “In your own words, what is a [conceptual/mathematical] understanding?”. C = conceptual prompt. M = mathematical prompt. The following numbers (1-5) were used for organization purposes.

Participant	C-1	C-2	C-3	C-4	C-5	M-1	M-2	M-3	M-4	M-5
SE_D_135_D2	Intuition	SynCon				Symbols	Unpaired			
W_D_497_U1	Intuition	Unpaired				Symbols	Relationships	Algorithm		
W_D_294_A3	Diagram	Modeling				Modeling	Symbols			
NE_D_223_L8	Relationships	Diagram	Apply	SynCon		SynMath	Relationships	Paired	Explain	Apply
MW_B_9_F6	Tool	Diagram	Explain	Unpaired	apply	Tool	Algorithm	Apply	Modeling	
W_D_470_I3	SynCon	Intuition	Symbols	Relationships		Symbols	Algorithm			
MW_B_363_M7	Explain	Word	Diagram			Symbols	Algorithm			
NE_B_282_U1	Apply	Explain	Intuition			Symbols	Relationships	Modeling		
MW_D_465_O3	Describe	Word	Intuition			Paired	Problem	Intuition	Algorithm	

Table 3.6: Percentages of Application of Individual Codes. These data show the percentage of application for each code, organized by associated prompt (“In your own words, what is [conceptual/mathematical] understanding?”). The total use column is the sum of the two category percentages.

Code Name	Conceptual Definition %	Mathematical Definition %	Total Use %	Code Name	Conceptual Definition %	Mathematical Definition %	Total Use %
Intuition	10.0	3.3	13.3	*Unpaired*	2.1	1.0	3.1
Symbols	0.8	11.9	12.7	*Diagram*	2.2	0.7	2.9
SynCon	6.6	1.4	7.9	*Word*	2.4	0.3	2.7
Explain	4.9	2.0	6.9	*Tool*	0.1	1.7	1.8
Relationships	3.5	3.2	6.6	*Describe*	1.1	0.4	1.6
Algorithm	0.0	6.2	6.2	*Error404*	0.6	0.6	1.1
Modeling	2.1	3.0	5.2	*Interpret*	0.1	0.8	0.9
Predict	2.3	2.5	4.8	*Memorization*	0.4	0.3	0.7
Paired	1.5	2.9	4.3	*Simplify*	0.5	0.2	0.7
Apply	2.0	2.1	4.1	*Generate*	0.0	0.7	0.7
SynMath	0.2	3.9	4.1	*Teach*	0.6	0.0	0.6
Transfer	2.7	0.7	3.5	*Argument*	0.1	0.3	0.4
Problem	1.4	2.0	3.5				

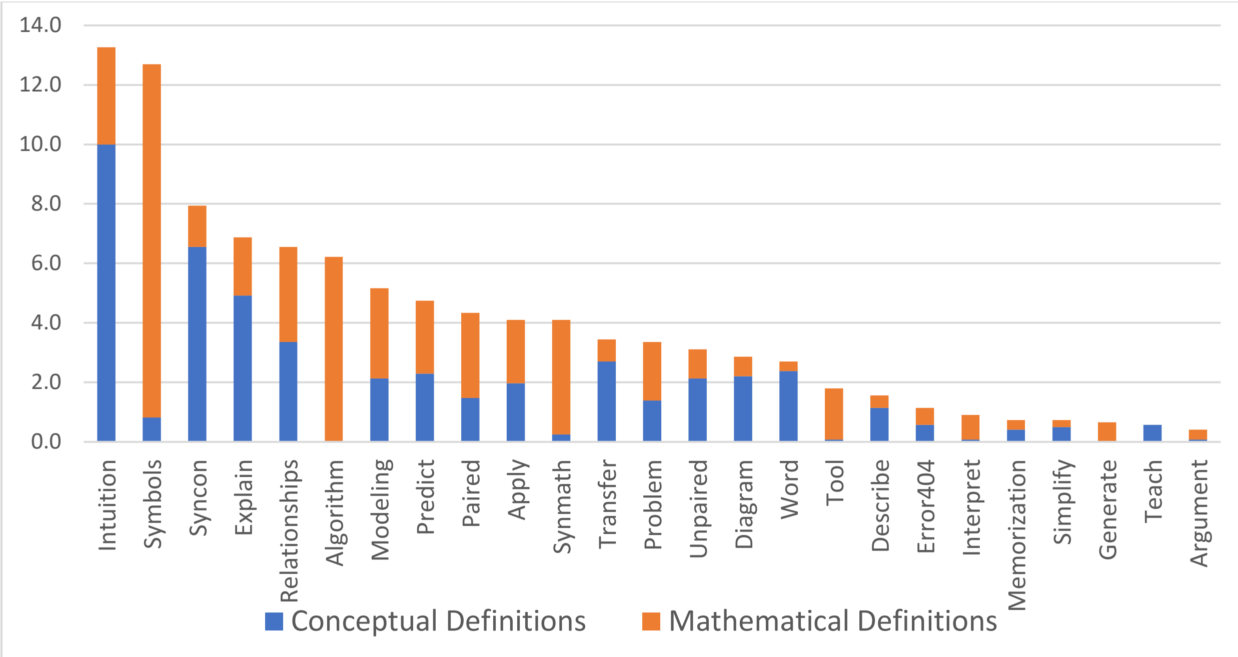

Figure 3.4: Percentage of Code Application by Knowledge Domain. These data show the percentage application of individual codes distributed between the two prompts ("In your own words, what is [conceptual/mathematical] understanding?"). E.g., the left most column indicates that ~13% percent of the total codes applied were the code "Intuition" (~10% being applied to participant's definition of "Conceptual Knowledge" and ~3% applied to participant's definitions of "Mathematical Knowledge").

The codes Relationships, Predict, Apply, and Error404 were applied evenly between the two knowledge domains (between 45%-55%). Table 3.7 shows a list depicting which knowledge domain codes were predominantly applied to. In addition to raw totals of code application, code data were processed by evaluating how they were applied to participants of differing research backgrounds. It was suspected (from personal experience) that research specialization may influence one's definitions of the two proposed knowledge domains. Research specializations were self-reported and binned as "Experimental", "Theoretical/Computational", "Physical Chemistry Education", and "Does Not Perform Research" (participants were allowed to select any combination of these bins, excluding combinations including "Does Not Perform Research").

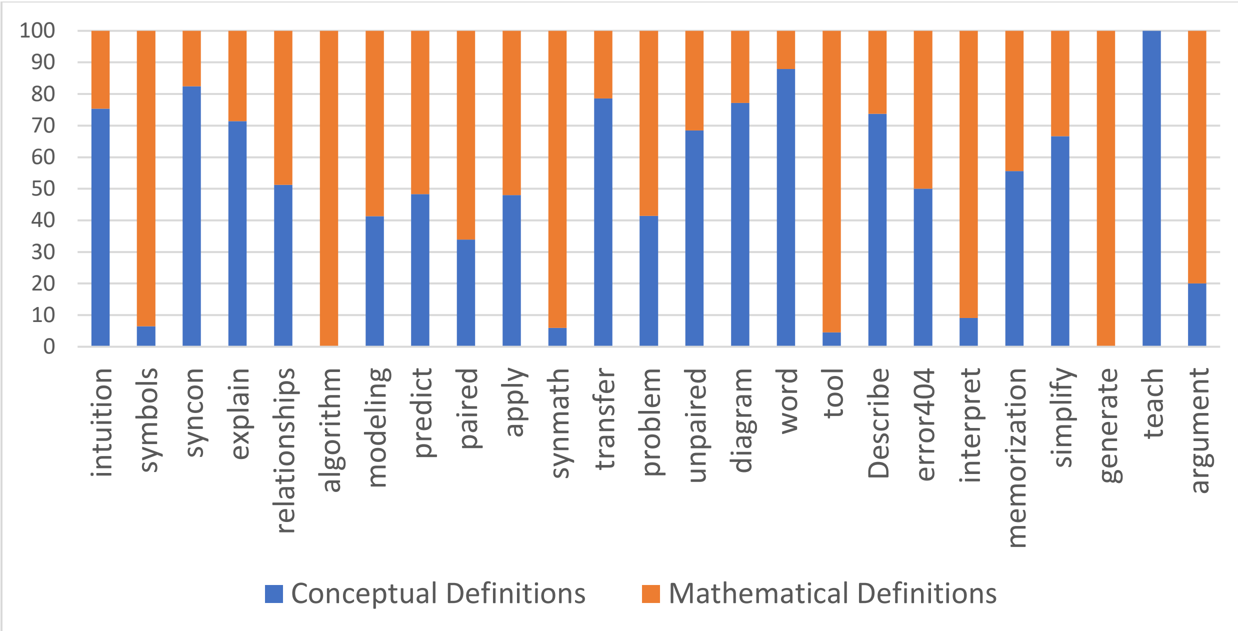

Figure 3.5: Normalized Percentage of Code Application by Knowledge Domain. This figure shows a normalized percentage distribution of each code as it was applied to the two prompts ("In your own words, what is [conceptual/mathematical] understanding?").

Table 3.7: Codes Grouped by Dominant Assignment of Knowledge Domain. This table shows the knowledge domain prompt to which codes are were most often applied. Placement in a category indicates the code was applied to that knowledge domain more than 55% of the time. The "Evenly Distributed" bin was reserved for codes whose distributions were between 45% and 55% in each domain.

Conceptual Leaning	Mathematical Leaning	Evenly Distributed
Intuition	Symbols	Relationships
SynCon	Algorithm	Predict
Explain	SynMath	Apply
Transfer	Problem	Error404
Unpaired	Tool	
Diagram	Interpret	
Word	Generate	
Describe	Paired	
Simplify	Modeling	
Teach		
Argument		
Memorization		

Figure 3.6 shows the percentage distribution of codes applied to participants of varying demographic. To make clearer the distribution of codes within these demographics, a normalized version of these data is provided in Figure 3.7.

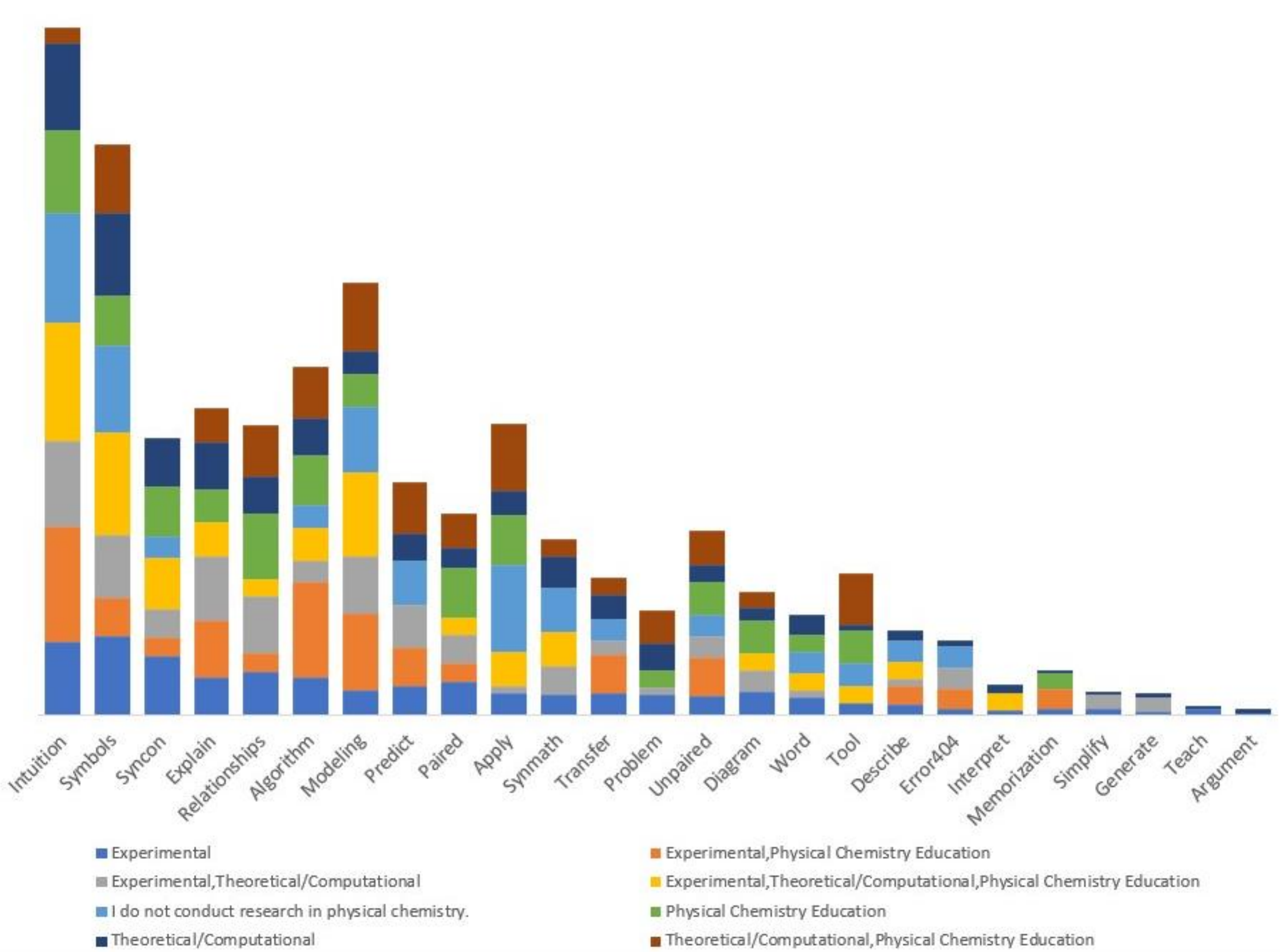

Figure 3.6: Percentage of Codes Applied to Individual Research Demographics. These data show the percentages of codes applied to participants who self-reported a description of their research specialization. Axis titles have been omitted as the relative percent proportions of codes applied to each demographic are the focus of this figure.

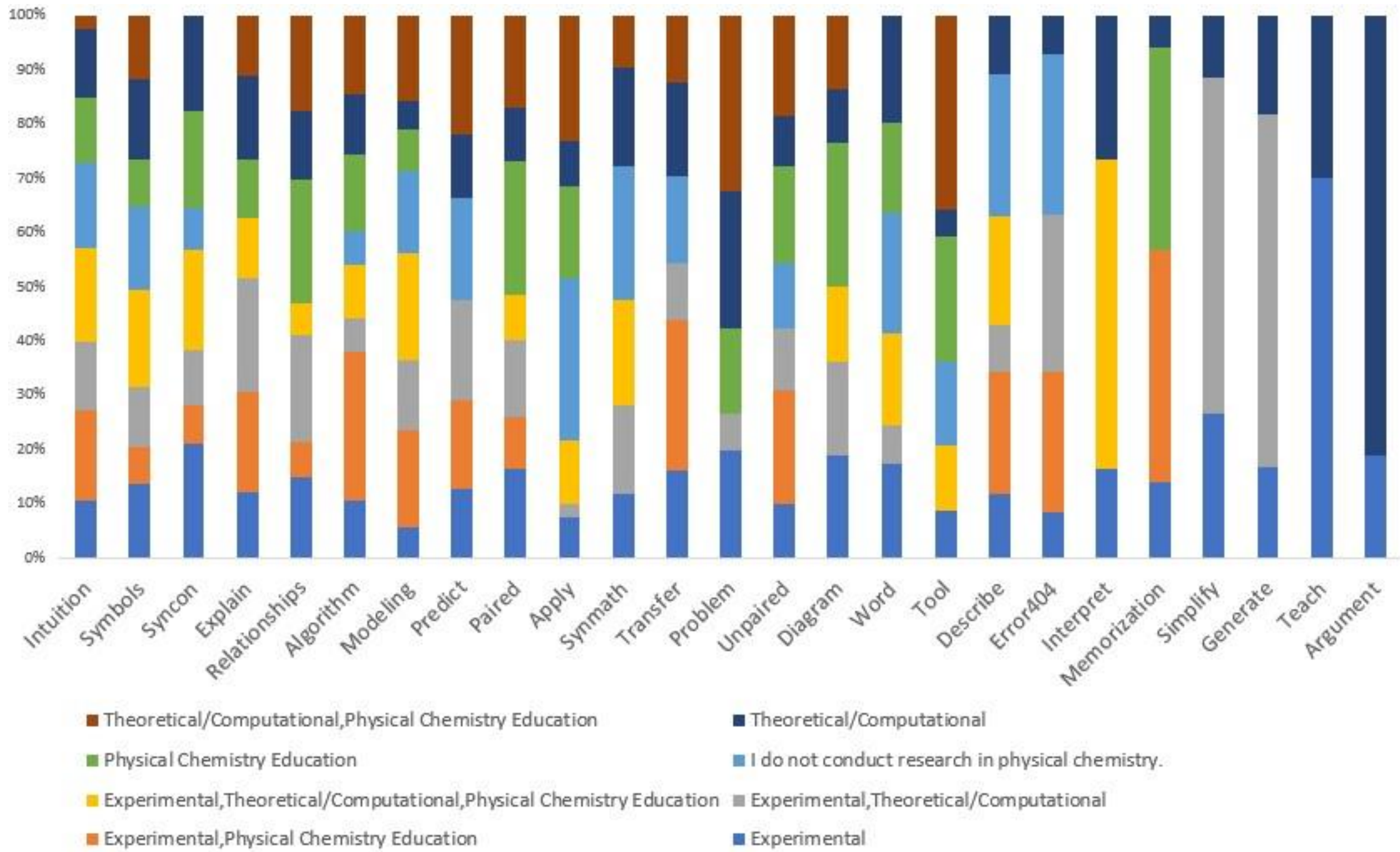

Figure 3.7: Normalized Percentage of Codes Applied to Individual Research Demographics. These data show a normalized representation of codes applied to participants of differing research specializations. The data appear to indicate, subjectively, an even distribution of codes between demographic, except for: Interpret, Memorization, Simplify, Teach, and Argument.

Subjectively, Figure 3.7 seems to indicate that the codes Interpret, Memorization, Simplify, Teach, and Argument are disproportionately represented by the groups "Experimental, Theoretical/Computational, Physical Chemistry Education", "Physical Chemistry Education" and "Experimental, Physical Chemistry Education", "Experimental, Theoretical/Computational", "Experimental", and "Theoretical/Computational", respectively. Statical analysis was necessary to make any conclusions about these distributions. To perform this analysis, the textual code data for each participant (previously shown in Table 3.5) was transcribed into a numerical form using Excel's "COUNTIF" function with the individual code names as search queries. A sample of the resulting numeric data is shown in Table 3.8. In Table 3.8, a value of "1" indicates that the code shown in the column heading was applied to either the conceptual or mathematical knowledge domain. A value of "2" indicates that the code was applied to both knowledge domains. The numeric data shown in Table 3.8 was analyzed using one-way ANOVA statistics, in SPSS. ANOVA analysis is like a student's t-test in that it can detect statistical variation in the means of multiple data sets, with the added benefit that it may operate on more than two datasets, simultaneously (a limitation of ANOVA analysis is that it may only indicate that one *or more* of the groups analyzed is statistically different. Independent t-tests must therefore be performed to determine *which* of the group(s) is the source of the variation). To perform iterative t-testing, the desired probability threshold for rejection of the null hypothesis must be adjusted to account for the inherent compounding of type one error[44]. This adjustment is performed by dividing the desired probability threshold (0.05 in our study) by the number of tests which are to be performed.

TABLE 3.8: Conversion of Applied Codes to Numerical Values. This table shows the conversion of textual data documenting our code application by knowledge domain prompt into numerical data. The numeric data was used to statistically analyze the application of codes by research demographic.

Participant	C-1	C-2	C-3	C-4	C-5	M-1	M-2	M-3	M-4	M-5
SE_D_135_D2	Intuition	SynCon				Symbols	Unpaired			
W_D_497_U1	Intuition	Unpaired				Symbols	Relationships	Algorithm		
W_D_294_A3	Diagram	Modeling				Modeling	Symbols			
NE_D_223_L8	Relationships	Diagram	Apply	SynCon		SynMath	Relationships	Paired	Explain	Apply
MW_B_9_F6	Tool	Diagram	Explain	Unpaired	Apply	Tool	Algorithm	Apply	Modeling	
W_D_470_I3	SynCon	Intuition	Symbols	Relationships		Symbols	Algorithm			
MW_B_363_M7	Explain	Word	Diagram			Symbols	Algorithm			
NE_B_282_U1	Apply	Explain	Intuition			Symbols	Relationships	Modeling		
MW_D_465_O3	Describe	Word	Intuition			Paired	Problem	Intuition	Algorithm	

Participant	Symbols	Diagram	Word	Explain	Teach	Modeling	Argument	Interpret	Problem	Simplify	Describe
SE_D_135_D2	1	0	0	0	0	0	0	0	0	0	0
W_D_497_U1	1	0	0	0	0	0	0	0	0	0	0
W_D_294_A3	1	1	0	0	0	2	0	0	0	0	0
NE_D_223_L8	0	1	0	1	0	0	0	0	0	0	0
MW_B_9_F6	0	1	0	1	0	1	0	0	0	0	0
W_D_470_I3	0	0	0	0	0	0	0	0	0	0	0
MW_B_363_M7	2	0	0	0	0	0	0	0	0	0	0
NE_B_282_U1	1	1	1	1	0	0	0	0	0	0	0
MW_D_465_O3	1	0	0	1	0	1	0	0	0	0	0
MW_D_465_O3	0	0	1	0	0	0	0	0	1	0	1
MW_B_682_R2	0	0	0	0	0	0	0	0	0	0	0

For example, we compared eight demographic bins, resulting in twenty-eight independent pairs to be analyzed (demographic 1,2; 1,3; 1,4 etc.). Thus, the appropriate probability threshold becomes 0.05 / 28 = 0.002. Our analysis indicated that of the twenty-five codes, only three showed statistical evidence of variation in their mean application between research demographics. These findings are reported in Table 3.9. The codes showing statistical variation were Modeling, Apply, and Tool. For the three codes showing statistical variation, independent student t-tests were performed to determine what, if any, relationship existed between these codes and the research specialization of the participant. The results of this analysis are provided in Table 3.10. In Table 3.10, when the calculated probability threshold is not attained ($p < 0.002$) the null hypothesis is rejected and there is statistical evidence that the code being referenced in the heading (grey bar) was applied differently between the demographics noted in the numerical pairings.

TABLE 3.9: One-way ANOVA Analysis of Codes Applied by Research Demographic. P-values less than 0.05 show a statistically significant difference (at the 95% confidence level) in the application of a code between one or more of the research demographics analyzed.

Code Name	n	Probability	F Value	η^2	Code Name	n	Probability	F Value	η^2
Symbols	155	0.641	0.737	0.021	Relationships	80	0.483	0.931	0.027
Diagram	35	0.641	0.737	0.021	Intuition	162	0.428	1.005	0.029
Word	33	0.917	0.374	0.011	Apply	50	0.004	3.112	0.084
Explain	84	0.721	0.642	0.018	Generate	8	0.713	0.652	0.019
Teach	7	0.863	0.460	0.013	Transfer	42	0.786	0.563	0.016
Modeling	63	0.007	2.859	0.077	SynCon	97	0.353	1.116	0.032
Argument	5	0.920	0.368	0.011	Memorization	9	0.517	0.887	0.025
Interpret	11	0.801	0.543	0.016	Paired	53	0.392	1.058	0.030
Problem	41	0.543	0.855	0.024	Unpaired	38	0.560	0.834	0.024
Simplify	9	0.641	0.736	0.021	Tool	22	0.002	3.379	0.090
Describe	19	0.925	0.360	0.010	SynMath	50	0.513	0.893	0.025
Predict	58	0.429	1.004	0.029	Error404	14	0.438	0.992	0.028
Algorithm	76	0.086	1.810	0.050	-		-	-	

Table 3.10: Independent T-test Analysis of Demographics with Different Means Via ANOVA. These data show iterative t-tests comparing the mean application of codes to participants of varying research specializations. Values below a calculated probability threshold of 0.002 (red) show statistical evidence (at the 95% confidence level) to reject the null hypothesis, indicating the codes noted in the corresponding heading (grey) were applied to the noted demographic pair (1-8) differently. Variance equality was calculated for each demographic using SPSS.

Modeling (Unequal Variance)													
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	0.318	2,3	0.644	3,4	0.583	4,5	0.025	5,6	0.335	6,7	0.581	7,8	0.171
1,3	0.211	2,4	0.935	3,5	0.624	4,6	0.331	5,7	0.159	6,8	0.264	-	-
1,4	0.151	2,5	0.895	3,6	0.551	4,7	0.134	5,8	0.668	-	-	-	-
1,5	0.177	2,6	0.436	3,7	0.175	4,8	0.712	-	-	-	-	-	-
1,6	0.659	2,7	0.298	3,8	0.426	-	-	-	-	-	-	-	-
1,7	0.736	2,8	0.818	-	-	-	-	-	-	-	-	-	-
1,8	0.183	-	-	-	-	-	-	-	-	-	-	-	-
Apply (Unequal Variance)													
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	<0.001	2,3	0.331	3,4	0.470	4,5	0.259	5,6	0.458	6,7	0.449	7,8	0.279
1,3	0.083	2,4	0.351	3,5	0.117	4,6	0.654	5,7	0.017	6,8	0.538	-	-
1,4	0.785	2,5	0.099	3,6	0.261	4,7	0.807	5,8	1.000	-	-	-	-
1,5	0.172	2,6	0.200	3,7	0.075	4,8	0.355	-	-	-	-	-	-
1,6	0.435	2,7	<0.001	3,8	0.204	-	-	-	-	-	-	-	-
1,7	0.904	2,8	0.178	-	-	-	-	-	-	-	-	-	-
1,8	0.274	-	-	-	-	-	-	-	-	-	-	-	-
Tool (Unequal Variance)													
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	0.001	2,3	*	3,4	0.351	4,5	0.760	5,6	0.760	6,7	0.253	7,8	0.242
1,3	0.001	2,4	0.351	3,5	0.374	4,6	0.486	5,7	0.501	6,8	0.504	-	-
1,4	0.845	2,5	0.374	3,6	0.172	4,7	0.580	5,8	0.406	-	-	-	-
1,5	0.643	2,6	0.172	3,7	0.025	4,8	0.311	-	-	-	-	-	-
1,6	0.354	2,7	0.025	3,8	0.208	-	-	-	-	-	-	-	-
1,7	0.206	2,8	0.208	-	-	-	-	-	-	-	-	-	-
1,8	0.279	-	-	-	-	-	-	-	-	-	-	-	-

P = 0.05/28 = 0.002

1 = Experimental, 2 = Experimental/Physical Chemistry Education, 3 = Experimental/Theoretical/Computational, 4 = Experimental/Theoretical/Computational/Physical Chemistry Education, 5 = Does not Perform Research, 6 = Physical Chemistry Education, 7 = Theoretical/Computational 8 = Theoretical/computational/Physical Chemistry Education

*No datapoints in selected group

As shown in Table 3.10, the code Modeling was found to have no statistical variation between individual groups (contrary to the previous ANOVA analysis – the small effect sizes noted in the ANOVA analysis, and the inherent difference between these the two statistical methods are likely the source of this discrepancy), and the codes Apply and Tool were shown to have only two groups (of twenty-eight possible pairs) showing evidence of variation. From these data, no conclusions may be drawn regarding *why* the noted demographics had the codes Apply and Tool applied different; however, based on the infrequency of variation, it is unlikely that any such relationship exists. It appears there is no meaningful difference in the way codes were applied to individuals of varying research specializations. Let us now transition to the quantitative portion of the FPPQMA data.

3.5: QUANTITATIVE DATA. Quantitative data from the FPPQMA survey were exported from Qualtrics to Microsoft Excel. The data were processed in Excel for subsequent statistical analysis using SPSS. In Excel, textual columnar data representing respondents' assignments of knowledge domain ("Mostly Conceptual", "Mostly Mathematical", etc.) were converted to numeric data using Excel's "COUNTA" function. A sample of binary data representing participant's knowledge domain assignments is shown in Table 3.11. In the Table 3.11, a value of "1" represents a respondent's section the knowledge domain corresponding to the column heading, while a value of "0" indicates that the respondent did not select the associated knowledge domain. For each survey each item (1-20), these data were summed by column yielding the total percentages of knowledge domain assignments shown in Figure 3.8. The data in Figure 3.8 show that 54.1% of the total knowledge domain assignments were "Mostly Conceptual", 29.4% were "Equally Conceptual and Mathematical", 11.9% were "Mathematical", and 4.6% were "Other". Using Microsoft Excel, Students t-tests were performed (calibrating the probability threshold for accurate comparison of iterative test results[44]) which compared the averages of each knowledge domain total shown in Figure 3.8. The results indicated that, at the 95% confidence level, the knowledge domain means are statically different. These data are reported in Table 3.12.

Table 3.11: Sample Binary Data Representing Participants Knowledge Domain Assignments. These data show individual respondent assignments of knowledge domain for item number 1 on the FPPQMA. A value of “1” indicates the respondent’s assignment was that corresponding to the column heading. A value of “0” indicates the respondent did not select the associated knowledge domain. Rows of 0 indicate that participant did not receive the survey item.

Participant	Mostly Conceptual	Mostly Mathematical	Equally Conceptual & Mathematical	Other
SE_D_135_D2	0	0	0	0
W_D_497_U1	0	0	0	0
W_D_294_A3	0	0	0	0
NE_D_223_L8	0	0	0	1
MW_B_9_F6	0	0	0	0
MW_B_238_M5	1	0	0	0
W_D_470_I3	0	0	0	0
MW_B_363_M7	0	0	0	0
NE_B_282_U1	0	0	0	0
MW_D_465_O3	0	0	0	0
MW_B_682_R2	0	0	0	0
SW_D_408_W5	1	0	0	0

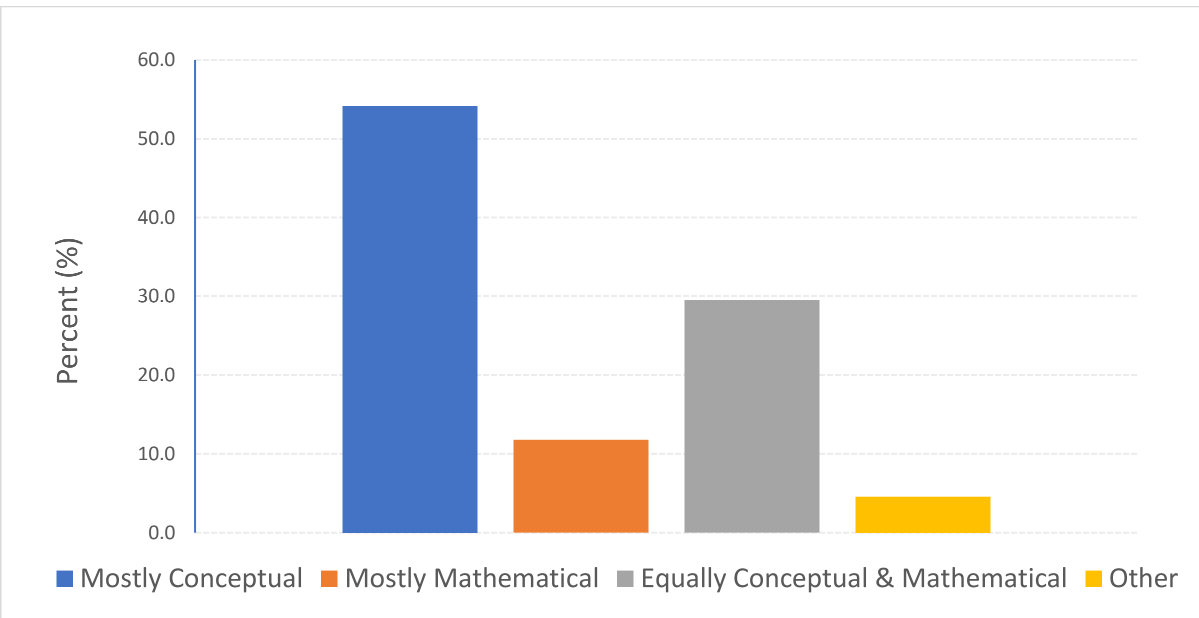

Figure 3.8: Total Percent of Knowledge Domain Assignment. These data show the total percentage of assignment for each knowledge domain (“Mostly Conceptual” “Mostly Conceptual” etc.) applied by respondents of the FPPQMA. Results: 54.1% “Mostly Conceptual”, 29.4% “Equally Conceptual and Mathematical”, 11.9% “Mathematical”, 4.6% “Other”.

Table 3.12: T-Test Results for Total Knowledge Domain Assignments. These data indicate that, at the 95% confidence level, the total number of times participants of this survey applied the four knowledge domains are statistically distinct. A calibrated p value[44] of 0.008 was used as the threshold to reject the null hypothesis.

Group	p	Group	p	Group	p
1,2	< 0.001	2,3	< 0.001	3,4	< 0.001
1,3	< 0.001	2,4	< 0.001		
1,4	< 0.001				

1 = Mostly Conceptual 2 = Mostly Mathematical 3 = Equally Conceptual and Mathematical 4 = Other

Figure 3.9 Shows the percentages of knowledge domain assignment organized by survey item. The data indicated that 13 of the 20 survey items received "Mostly Conceptual" as the dominant knowledge domain assignment (determined by the largest percentage of knowledge domain section). Item 2 was the only survey item which received "Mostly Mathematical" as the majority assignment. Items 12 and 18 show, qualitatively, an even distribution of knowledge domain assignments. Questions 7, 8, and 16 were found to have "Equally Conceptual and Mathematical" as the dominant knowledge domain assignment. To address research question 1, "*How do physical chemistry instructors view the nature of questions in QM concept inventories?*" and research aim 3, "*Evaluate the impact surface level features of question design (use of images, graphs, symbols etc.) have on physical chemistry educators' conceptualizations of assessment materials*" respondent assignments of knowledge domain were sorted by the representational form used in the survey item and by the ACS topic that best described the content of question. Figure 3.10 shows the percentage of knowledge domain assignments when respondent data was grouped by ACS Topic. With the exclusion of the ACS Topic "Wave-Particle Duality", these data indicated that the majority knowledge domain assignment was "Mostly Conceptual", regardless of which ACS topic best described the survey item.

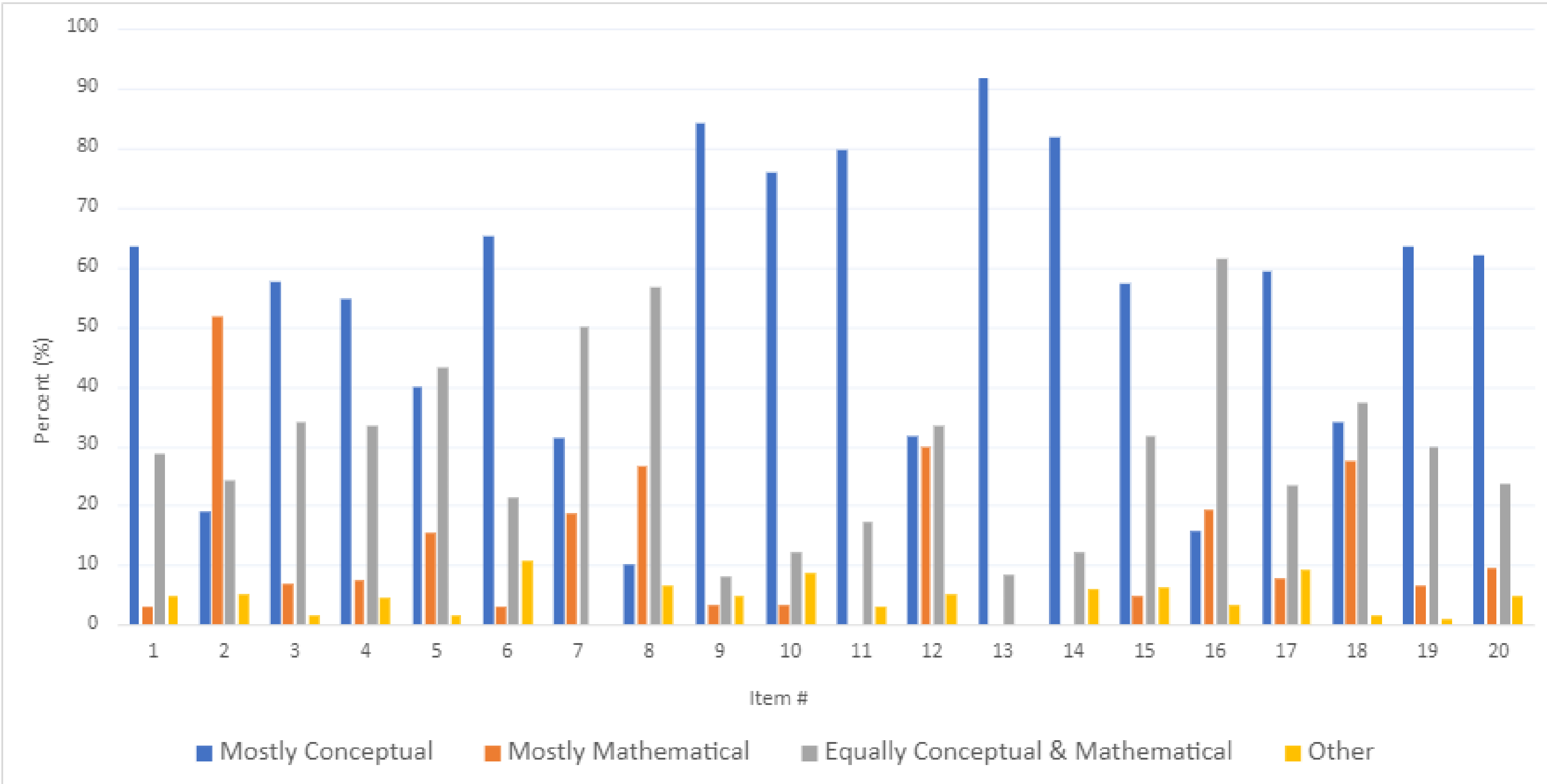

Figure 3.9: Percent of Knowledge Domain Assignment by Question. These data show the percentages of knowledge Assignment of respondents to the FPPQMA, organized by item number.

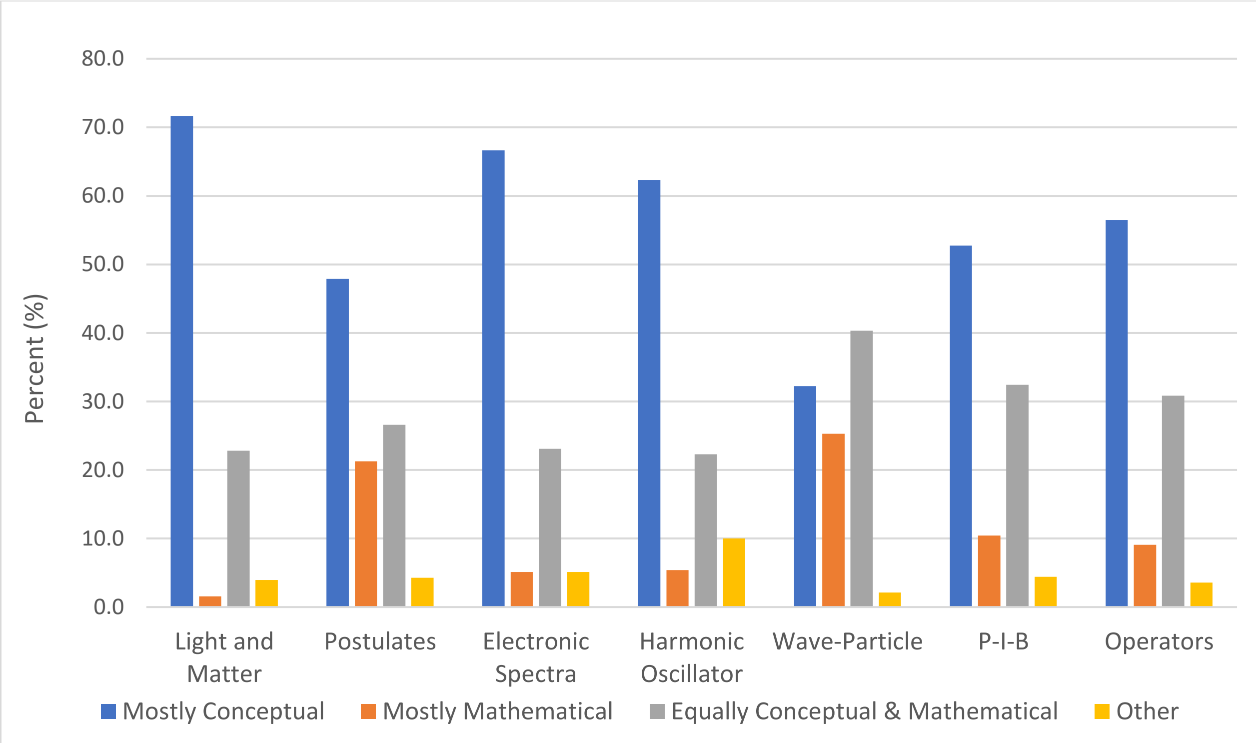

Figure 3.10: Percent of Knowledge Domain Assignments by ACS Topic. This figure shows the percentage of assignment of knowledge domain ("Mostly Conceptual", "Mostly Conceptual", etc.) when respondent data is grouped by the ACS topics used to describe the content of the survey items.

Wave-Particle Duality questions were found to be predominantly categorized by participants as "Equally Conceptual and Mathematical." These data were statistically analyzed by comparing the individual knowledge domain means for survey items of varying ACS Topics (i.e., comparing how many participants selected "Mostly Conceptual" "Mostly Mathematical" etc. to questions with different ACS topics). One-way ANOVA analysis revealed that, at the 95% confidence interval, the knowledge domain assignment means, compared between ACS Topics, were different (i.e., the mean assignment of "Mostly Conceptual", for example, varies between questions of varying ACS Topic); however, the correlation coefficients for these calculations was very small[43] suggesting the results may not be meaningful. Results from ANOVA analysis are provided in Table 3.13.

Table 3.13: One-Way ANOVA Analysis of Knowledge Domain Assignments by ACS Topic. These data indicate that, at the 95% confidence level, there is a statistical difference between the mean assignment of knowledge domains when compared between different ACS topics ($p < 0.05$).

Knowledge Domain	n	Probability	F	η^2
Mostly Conceptual	653	<0.001	6.135	0.007
Mostly Mathematical	162	<0.001	9.837	0.011
Equally Mathematical & Conceptual	369	0.016	2.593	0.003
Other	56	0.049	2.108	0.002

Subsequent t-test analysis was performed to determine which of the ACS Topic groups was responsible for the noted variation. T-test results are shown in Table 3.14**.** The results found in Table 3.14 indicate that there are no groups showing statical variation for the "Equally Conceptual and Mathematical" and "Other" Knowledge domains. This conflicts with the results of ANOVA analysis; however, it is believed this is the result of the very small effect sizes[43] previously shown in Table 3.13. The knowledge domain "Mostly Conceptual" was found to have 6 of 21 groups showing statistical variation, and the knowledge domain "Mostly Mathematical" had 9 of 21 groups. These results show no clear patter which can be used to draw conclusions regarding a relationship between the ACS-topic of a survey item and the knowledge domain selected by the participant. Further, this type of analysis cannot provide causal rational for the observed variation. Follow-up interviews will be necessary to determine the cause of variation. Additionally, given the very small effect sizes[43], these results are not thought likely to indicate a meaningful relationship between ACS topic and knowledge domain assignment.

Figure 3.11 shows the percentage of knowledge domain assignment when respondent data was grouped by representational form. As shown in Figure 3.11, the predominant knowledge domain assignment was "Mostly Conceptual", regardless of the representational form used in the survey item. These data were statistically analyzed by comparing the individual selected knowledge domains across survey items with differing representational forms.

Table 3.14: T-Testing of Knowledge Domain Assignments by ACS Topic Group. These data indicate the ACS Topic groups which show statistical variation (p = 0.05 / 21 = 0.002) in red.

Mostly Conceptual (Unequal Variance)											
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	0.002	2,3	0.075	3,4	0.796	4,5	<0.001	5,6	0.002	6,7	0.876
1,3	0.275	2,4	0.040	3,5	<0.001	4,6	0.099	5,7	<0.001	-	-
1,4	0.404	2,5	0.010	3,6	0.170	4,7	0.056	-	-	-	-
1,5	<0.001	2,6	0.639	3,7	0.106	-	-	-	-	-	-
1,6	0.011	2,7	0.819	-	-	-	-	-	-	-	-
1,7	0.004	-	-	-	-	-	-	-	-	-	-
Mostly Mathematical (Unequal Variance)											
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	<0.001	2,3	<0.001	3,4	0.780	4,5	<0.001	5,6	<0.001	6,7	0.329
1,3	0.156	2,4	<0.001	3,5	<0.001	4,6	0.146	5,7	0.003	-	-
1,4	0.094	2,5	0.440	3,6	0.077	4,7	0.010	-	-	-	-
1,5	<0.001	2,6	0.005	3,7	0.003	-	-	-	-	-	-
1,6	<0.001	2,7	0.033	-	-	-	-	-	-	-	-
1,7	<0.001	-	-	-	-	-	-	-	-	-	-
Equally Conceptual & Mathematical (Unequal Variance)											
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	0.538	2,3	0.353	3,4	0.784	4,5	0.006	5,6	0.148	6,7	0.915
1,3	0.784	2,4	0.533	3,5	0.002	4,6	0.151	5,7	0.136	-	-
1,4	1.000	2,5	0.020	3,6	0.081	4,7	0.091	-	-	-	-
1,5	0.006	2,6	0.372	3,7	0.041	-	-	-	-	-	-
1,6	0.151	2,7	0.264	-	-	-	-	-	-	-	-
1,7	0.091	-	-	-	-	-	-	-	-	-	-
Other (Unequal Variance)											
Group	p	Group	p	Group	p	Group	p	Group	p	Group	p
1,2	0.909	2,3	0.828	3,4	0.105	4,5	0.006	5,6	0.247	6,7	0.819
1,3	0.762	2,4	0.057	3,5	0.230	4,6	0.057	5,7	0.266	-	-
1,4	0.057	2,5	0.274	3,6	0.828	4,7	0.032	-	-	-	-
1,5	0.369	2,6	1.000	3,7	0.668	-	-	-	-	-	-
1,6	0.909	2,7	0.819	-	-	-	-	-	-	-	-
1,7	0.939	-	-	-	-	-	-	-	-	-	-

1 = Light & Matter, 2 = Postulates, 3 = Electronic Spectra, 4 = Harmonic Osc. 5 = Wave/Particle, 6 = P-I-B, 7 = Operators

One-way ANOVA analysis revealed that, at the 95% confidence level, there is a statistically significant difference between knowledge domains selected for questions of different representational form (i.e., the mean assignment of “Mostly Conceptual”, for example, varies between questions of differing representational form). Results from this ANOVA analysis are provided in Table 3.15. Again, the effect sizes for each analysis were found to be very small[43].

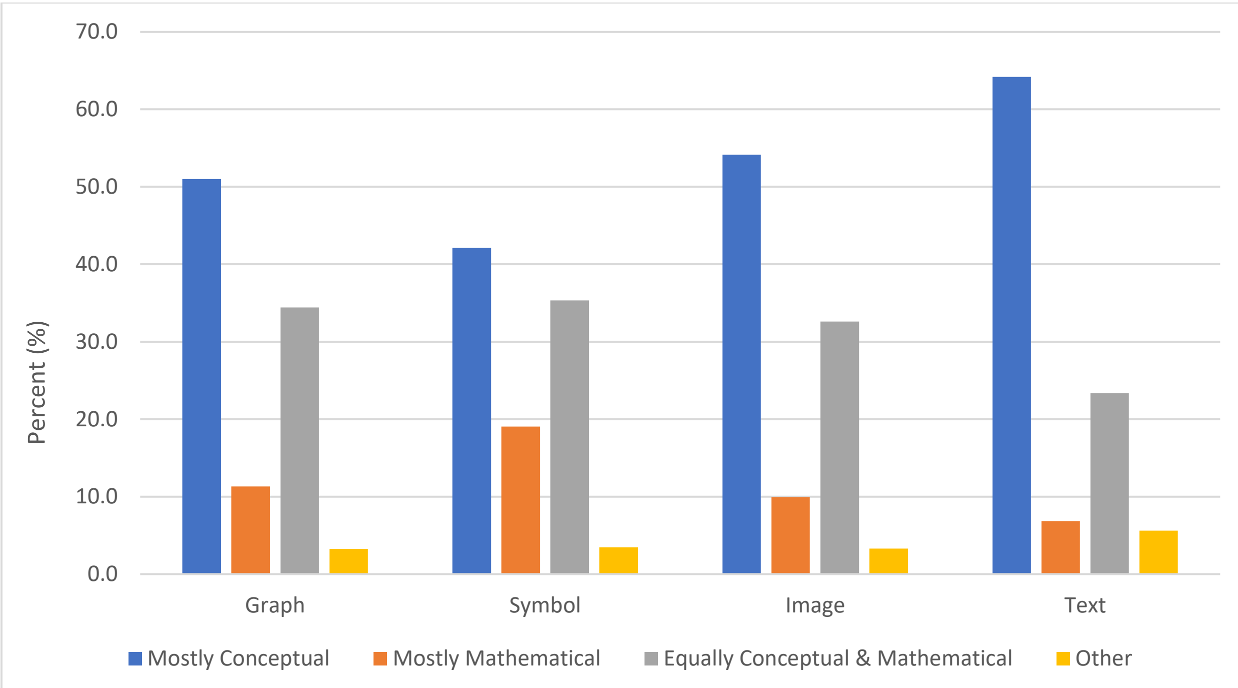

Figure 3.11: Percent of Knowledge Domain Assignments by Representational Form. This figure shows the percentage of application of knowledge domains ("Mostly Conceptual", "Mostly Mathematical", etc.) when respondent data is grouped by representational form (graphical, textual, symbolic, or image).

Table 3.15: One-Way ANOVA Analysis of Knowledge Domain by Representation Form. These data indicate that at the 95% confidence level there is statistical difference ($p < 0.05$) between 3 of the 4 groups of representational form. mean values of knowledge domain application when participant responses are sorted by the representational form used in the concept inventory question.

Knowledge Domain	n	Probability	F Value	η^2
Mostly Conceptual	745	<0.001	8.394	0.004
Mostly Mathematical	155	<0.001	9.652	0.005
Equally Mathematical & Conceptual	396	0.018	3.348	0.002
Other	60	0.131	1.879	0.001

Table 3.16 shows iterative t-tests performed to determine which of the groups was responsible for the observed variation. As was found to be the case with ACS-topic groups, representational form groupings showed no discernable pattern that could be used to draw conclusions regarding a relationship between the representational form of questions and the knowledge domain selected by participants. Again, follow-up interviews are necessary to determine the cause of the observed, albeit minor, variation between representational form groupings.

Table 3.16: T-Testing of Knowledge Domain Assignments by Representational Form. These data indicate the representational form pairings which show statistical variation ($p < 0.05 / 6 = 0.008$) in red.

Mostly Conceptual (Unequal Variance)					
Group	*p*	*Group*	*p*	*Group*	*p*
1,2	0.178	*2,3*	0.113	*3,4*	0.029
1,3	0.732	*2,4*	<0.001	-	-
1,4	0.004	-		-	-
Mostly Mathematical (Unequal Variance)					
Group	*p*	*Group*	*p*	*Group*	*p*
1,2	0.014	*2,3*	0.004	*3,4*	0.285
1,3	0.599	*2,4*	<0.001	-	-
1,4	0.070	-		-	-
Equally Conceptual & Mathematical (Unequal Variance)					
Group	*p*	*Group*	*p*	*Group*	*p*
1,2	0.653	*2,3*	0.912	*3,4*	0.077
1,3	0.628	*2,4*	0.015	-	-
1,4	0.011	-		-	-
1 = Graphical, 2 = Symbolic, 3 = Image 4 = Textual					

The FPPQMA knowledge domain data was further analyzed for the influence that a host of personal demographics might have on physical chemistry experts' beliefs. This analysis was used to determine if factors outside of a survey item's content and/or representational form could influence a participants' response. The demographics studied were the US Region of the participant's university, the highest degree offered by participant's university, the Carnegie classification of the participant's university, the type of research performed by the participant, the last time the participant taught physical chemistry, and how many times the participant had taught a physical chemistry course. Table 3.17 shows a list of all demographics and the associated bins used in this study. To perform this analysis, each participants' assignment of knowledge domain, per question, was converted into a singular value. Table 3.18 shows a sub-set of these data.

Table 3.17: Demographic Bins and Sub-Categories. This table shows the demographic bins used to analyze respondent data. For each demographic, the sub-categories used in this study have been provided.

US Region	Highest Degree	Carnegie Classification	Research Specialization	The Last Time Participant Taught Physical Chemistry	How Many Times Participant Taught Physical Chemistry
West	Bachelor's	R1	Experimental	Never	Never
Midwest	Master's	R2	Experimental, Theoretical/Computational	Within Last Year	1-5 Times
Southeast	Ph.D.	R3	Does Not Perform	1-5 Years	6-10 Times
Northeast	-	M1	Theoretical/Computational	6-10 Years	11-15 Times
Southwest	-	M2	Experimental, Physical Chemistry Education	11-15 Years	16-20 Times
-	-	M3	Experimental, Theoretical/Computational, Physical Chemistry Education	16-20 Years	More Than 20 Times
-	-	D/PU	Physical Chemistry Education	More Than 20 Years	-
-	-	Special Focus	Theoretical/Computational Physical Chemistry Education	-	-
-	-	Diverse Fields	-	-	-
-	-	Arts & Science	-	-	-

A value 1 was used to indicate that the participant applied the knowledge domain "Mostly Conceptual." A value of 2 indicates "Mostly Mathematical." A value of 3 indicates "Equally Mathematical and Conceptual." Finally, a value of 4 indicates "Other." The mean knowledge domain value of both the individual survey items ($\bar{x}$ columns 1-20 in Table 3.18) and the mean knowledge domain assignment per respondent ($\bar{x}$ rows in Table 3.18) were calculated and analyzed while controlling for a variety of demographics. A one-way ANOVA analysis of the knowledge domain assignments per individual survey item ($\bar{x}$ columns 1-20 in Table 3.18), grouped by the demographics noted in Table 3.17, revealed that, at the 95% confidence level, the majority of knowledge domain application per survey item showed no statistical difference.

Table 3.18: Integer Respondent Data Depicting Knowledge Domain Assignments. This figure shows a representation of integer data that represents each participants knowledge domain assignment to the 20 survey items. A value of 1 corresponds to the knowledge domain "Mostly Conceptual", 2 corresponds to "Mostly Mathematical", 3 to "Equally Conceptual and Mathematical", and 4 to "Other.

Participant	1	2	3	4	5	6	7	8	9	10	11	11	12	13	14	15	16	17	18	19	20
SE_D_135_D2	.	.	.	.	.	.	.	1	.	.	.	1	1	.	2	.	.	.	1	.	.
W_D_497_U1	.	.	.	.	3	.	.	.	1	2	2	.	.	.	.		.	.	.	.	.
W_D_294_A3		3	1	.	.		.	.	.	.	.	.	.	2	.	.	.	2	.	.	
NE_D_223_L8	.	.	.	2	.	.	2	.	.	.	.	.	.	.	1	2	.	1	.	.	.
MW_B_9_F6	1	.	.	.	2	.	.	.	1	.	1	.	1	.	.	.	.	.	.	.	1
MW_B_238_M5	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
W_D_470_I3	.	.	1	.	.	.	.	.	.	1	.	2	.	.	.	.	.	.	2	1	.
MW_B_363_M7	.	.	.	.	1	.	1	3	1	.	.	.	.	1	.	.	.	.	.	.	.
NE_B_282_U1	.	.	3	.	.	1	.	.	.	.	.	3	.	.	.	.	.	.	2	1	.
MW_D_465_O3	.	2	.	.	.	1	.	.	1	.	1	.	.	.	.	.	1	.	.	.	.

These data are reported in Table 3.19. However, exceptions were noted: Q8 analyzed by region, Q4 analyzed by Carnegie classification, Q10 analyzed by research specialization, Q6 & Q18 analyzed by the last time a participant taught physical chemistry, and Q5, Q6, Q10, Q15, and Q20 when analyzed by the number of times a participant taught a physical chemistry course. In response to ANOVA results which indicated the presence of more than one value showing statistical difference, independent t-tests were utilized to pinpoint the source of variation. Table 3.20 reports the results of multiple independent t-tests used to determine which means were unique by demographic. As was the case for ACS topic, and representational form, these analyses show no discernable trend which could be used to outline a relationship between the demographics examined in this study and the knowledge domain assignments of participants.

Table 3.19: One-Way AVOVA Analysis of Participant Responses, by Question, by Demographic. These data show the results of one-way ANOVA analysis of the mean values of each individual item on the FPPQMA. P values higher than 0.05 indicate that, at the 95% confidence level, no statistical difference exists between the means of each individual demographic sub-group, per question. Values shown in red are those for which the calculated p value is below the 0.05 threshold.

FPPQMA Item #	Probability	F	η^2	FPPQMA Item #	Probability	F Value	η^2
Grouped By Region							
1	0.568	0.741	0.049	*11*	0.455	0.926	0.059
2	0.179	1.636	0.110	*12*	0.862	0.322	0.023
3	0.610	0.678	0.048	*13*	0.516	0.823	0.057
4	0.926	0.221	0.015	*14*	0.288	1.281	0.079
5	0.777	0.443	0.029	*15*	0.633	0.645	0.043
6	0.702	0.547	0.035	*16*	0.259	1.365	0.095
7	0.209	1.517	0.095	*17*	0.847	0.344	0.023
8	0.825	0.376	0.027	*18*	0.405	1.020	0.067
9	0.251	1.385	0.089	*19*	0.466	0.908	0.060
10	0.642	0.632	0.046	*20*	0.978	0.111	0.008
Grouped By Highest Degree Offered by Participant's University							
1	0.102	2.371	0.073	*11*	0.423	0.873	0.028
2	0.458	0.793	0.028	*12*	0.643	0.445	0.015
3	0.336	1.112	0.038	*13*	0.268	1.348	0.046
4	0.643	0.445	0.014	*14*	0.422	0.874	0.027
5	0.961	0.04	0.001	*15*	0.913	0.091	0.003
6	0.367	1.019	0.032	*16*	0.203	1.641	0.057
7	0.895	0.111	0.004	*17*	0.454	0.800	0.026
8	0.004	6.001	0.174	*18*	0.417	0.888	0.029
9	0.498	0.705	0.023	*19*	0.641	0.447	0.015
10	0.366	1.024	0.036	*20*	0.566	0.574	0.019
Grouped By Carnegie Classification							
1	0.691	0.677	0.079	*11*	0.262	1.301	0.159
2	0.611	0.793	0.115	*12*	0.715	0.647	0.080
3	0.258	1.350	0.113	*13*	0.770	0.604	0.088
4	0.045	2.229	0.215	*14*	0.711	0.652	0.074
5	0.940	0.324	0.038	*15*	0.748	0.575	0.058
6	0.713	0.621	0.060	*16*	0.853	0.391	0.037
7	0.768	0.607	0.082	*17*	0.566	0.810	0.080
8	0.614	0.771	0.094	*18*	0.255	1.329	0.147
9	0.979	0.219	0.028	*19*	0.202	1.458	0.159
10	0.356	1.136	0.137	*20*	0.777	0.570	0.069
Grouped By Participant's Research Specialization							
1	0.549	0.853	0.098	*11*	0.481	0.910	0.073
2	0.918	0.365	0.049	*12*	0.330	1.182	0.118
3	0.510	0.889	0.093	*13*	0.792	0.518	0.056
4	0.696	0.642	0.062	*14*	0.561	0.817	0.078

5	0.867	0.370	0.030	*15*	0.990	0.143	0.015
6	0.299	1.235	0.132	*16*	0.866	0.415	0.047
7	0.927	0.349	0.043	*17*	0.583	0.788	0.078
8	0.179	1.527	0.170	*18*	0.714	0.619	0.063
9	0.785	0.527	0.054	*19*	0.481	0.929	0.092
10	0.010	3.014	0.297	*20*	0.927	0.314	0.033
Grouped By the Last Time Respondent Taught Physical Chemistry							
1	0.75	0.573	0.058	*11*	0.052	2.348	0.168
2	0.642	0.632	0.046	*12*	0.453	0.931	0.063
3	0.918	0.234	0.017	*13*	0.879	0.395	0.044
4	0.834	0.418	0.034	*14*	0.429	0.973	0.061
5	0.825	0.431	0.035	*15*	0.396	1.036	0.067
6	0.003	4.531	0.232	*16*	0.309	1.229	0.108
7	0.779	0.494	0.052	*17*	0.657	0.611	0.040
8	0.345	1.145	0.077	*18*	0.005	4.103	0.224
9	0.291	1.275	0.082	*19*	0.268	1.323	0.106
10	0.936	0.296	0.034	*20*	0.103	1.936	0.147
Grouped By How Many Times Respondent Has Taught Physical Chemistry							
1	0.800	0.466	0.039	*11*	0.364	1.113	0.088
2	0.220	1.458	0.123	*12*	0.865	0.373	0.033
3	0.945	0.236	0.022	*13*	0.658	0.656	0.094
4	0.763	0.516	0.042	*14*	0.312	1.218	0.094
5	0.016	3.064	0.206	*15*	0.030	2.695	0.191
6	0.010	3.368	0.222	*16*	0.523	0.847	0.077
7	0.813	0.448	0.038	*17*	0.805	0.459	0.039
8	0.285	1.284	0.106	*18*	0.924	0.276	0.024
9	0.446	0.966	0.079	*19*	0.815	0.445	0.038
10	0.046	2.44	0.190	*20*	0.017	3.049	0.214

Table 3.20: Independent T-test Analysis of Demographics With Different Means Via ANOVA. These data show iterative t-tests between sub-groups within a demographic. The probability threshold of each group was adjusted to account for compounding type 1 error[44]. Values below the calculated probability threshold show a statistical difference in their means and are highlighted in red text. Variance equality was calculated for each demographic using SPSS.

Last Time Participant Taught Physical Chemistry: Q6 (Unequal Variance)											
Group	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*
1,2	0.002	2,3	0.076	3,4	0.567	4,5	*	5,6	*	6,7	*
1,3	0.062	2,4	0.714	3,5	*	4,6	*	5,7	*	-	-
1,4	0.137	2,5	*	3,6	*	4,7	*	-	-	-	-
1,5	*	2,6	*	3,7	*	-	-	-	-	-	-
1,6	*	2,7	*	-	-	-	-	-	-	-	-
1,7	*	-	-	-	-	-	-	-	-	-	-

Last Time Participant Taught Physical Chemistry: Q18 (Equal Variance)											
Group	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*
1,2	0.571	2,3	0.483	3,4	0.025	4,5	0.001	5,6	**	6,7	**
1,3	0.368	2,4	0.001	3,5	0.115	4,6	**	5,7	**	-	-
1,4	0.004	2,5	0.094	3,6	**	4,7	**	-	-	-	-
1,5	0.264	2,6	**	3,7	**	-	-	-	-	-	-
1,6	**	2,7	**	-	-	-	-	-	-	-	-
1,7	**	-	-	-	-	-	-	-	-	-	-

p = 0.05 / 21 = 0.002
1 = never, 2 = Within the last year, 3 = (1-5) Years ago, 4 = (6-10) Years ago, 5 = (11-15) Years ago, 6 = (16-20) Years ago, 7 = more than 20 years ago
**Group 6 and 7 did not have any data corresponding to item Q6.*
*** Group 6 and 7 did not have any data corresponding to item Q18.*

How Many Times a Participant Has Taught Physical Chemistry: Q5 (Unequal Variance)									
Group	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*
1,2	0.272	2,3	0.245	3,4	0.006	4,5	0.197	5,6	<0.001
1,3	0.094	2,4	0.033	3,5	<0.001	4,6	0.030	-	-
1,4	0.652	2,5	<0.001	3,6	0.539	-	-	-	-
1,5	0.304	2,6	0.686	-	-	-	-	-	-
1,6	0.203	-	-	-	-	-	-	-	-

How Many Times a Participant Has Taught Physical Chemistry: Q6 (Unequal Variance)									
Group	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*
1,2	0.001	2,3	0.317	3,4	0.769	4,5	0.182	5,6	0.040
1,3	0.003	2,4	0.733	3,5	0.002	4,6	0.556	-	-
1,4	0.020	2,5	0.047	3,6	0.654	-	-	-	-
1,5	0.003	2,6	0.279	-	-	-	-	-	-
1,6	0.051	-	-	-	-	-	-	-	-

How Many Times a Participant Has Taught Physical Chemistry: Q10 (Equal Variance)									
Group	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*
1,2	0.525	2,3	0.704	3,4	0.044	4,5	0.109	5,6	0.139
1,3	0.804	2,4	0.011	3,5	0.941	4,6	0.001	-	-
1,4	0.092	2,5	0.856	3,6	0.133	-	-	-	-
1,5	0.803	2,6	0.243	-	-	-	-	-	-
1,6	0.093	-	-	-	-	-	-	-	-

How Many Times a Participant Has Taught Physical Chemistry: Q15 (Unequal Variance)

Group	p	Group	p	Group	p	Group	p	Group	p
1,2	0.055	2,3	0.846	3,4	0.041	4,5	0.069	5,6	0.286
1,3	0.056	2,4	0.001	3,5	0.296	4,6	0.035	-	-
1,4	0.001	2,5	0.237	3,6	0.983	-	-	-	-
1,5	0.944	2,6	0.858	-	-	-	-	-	-
1,6	0.044	-	-	-	-	-	-	-	-
How Many Times a Participant Has Taught Physical Chemistry: 20 (Unequal Variance)									
Group	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*	*Group*	*p*
1,2	0.001	2,3	0.338	3,4	0.490	4,5	0.956	5,6	0.169
1,3	0.021	2,4	0.065	3,5	0.535	4,6	0.160	-	-
1,4	0.081	2,5	0.090	3,6	0.044	-	-	-	-
1,5	0.095	2,6	0.001	-	-	-	-	-	-
1,6	0.347	-	-	-	-	-	-	-	-

p = 0.05 / 15 = 0.003

1 = never, 2 = (1-5) times, 3 = (6-10) times, 4 = (11-15) times, 5 = (16-20) times, 6 = more than times

The average knowledge domain classification per respondent was calculated by the averaging the row values in Table 3.18, and analyzed using a one-way ANOVA, again, controlling for the demographics shown in Table 3.17. This analysis showed that, at the 95% confidence level, there is no statistical difference between the average knowledge domain classification of any participant throughout the survey, while controlling for the noted demographics. These data are shown in Table 3.21.

Table 3.21: One-way ANOVA Analysis of Average Knowledge Domain Rating. These data indicate that at the 95% confidence level there is no statistically significant difference between the mean application knowledge domain of any participant controlling for all noted demographics.

Controlled For:	Probability	F Value	η^2
Region	0.392	1.031	0.017
Highest Degree	0.485	0.727	0.006
Carnegie Classification	0.993	0.187	0.006
Research	0.996	0.130	0.004
Last Time Teaching Physical	0.191	1.464	0.035
How Many Times Teaching Physical	0.622	0.702	0.014

3.6: IMPORTANT CONCEPTS. Participants of the FPPQMA survey were asked to provide lists of the five most important concepts and five most important mathematical tools which they believed students of an undergraduate physical chemistry course should take away with them. We were surprised to find that much of the data was not simply a list of single words, or short phrases, but instead, long paragraph-form responses. A word count analysis was performed on the complete data set, regardless of whether it was clear how to demarcate the participants response into singular items. The function "=IFS([cell]>0,LEN([cell])-LEN(SUBSTITUTE([cell]," ",""))+1,[cell]="","")" was used to perform this task. The LEN component of this function returns the character count of the cell, and the SUBSTITUTE portion find the spaces between characters. The difference plus 1, then, is the number of groups with spaces between them. It should be noted that this function does not account of the use of symbols like dashes or hyphens, so the actual word counts are likely higher than those reported here. Table 3.22 shows a sample of these data. Once word counts were tabulated for each participant, averages were taken of the responses pertaining to concepts and to mathematical tools, individually. It was found that the average number of words it took participants to describe 5 concepts was 18.1, while the average word count to provide 5 mathematical tools was found to be 12.5 words. It took, on average, 5.6 more words to describe the important concepts than the important mathematical tools.

Table 3.22: Word Count Performed in Microsoft Excel. These data show a sample of the document used to determine the word count of each participants response to the 5 most important concepts and the 5 most important mathematical tools that physical chemistry students should take aways from undergraduate classrooms.

Participant	Conceptual	Words	Mathematical	Words
SE_D_135_D2	"MO Theory, Approximate Methods (variational in particular), origin of quantum numbers, origin of quantum phenomena"	15	"Eigenfunctions/eigenvalues"	1
W_D_497_U1	"The most important concept is the idea of the duality of nature and that the classical world in which we live our every day lives is a limiting case of the more complex actual world. Furthermore, in the actual world there are limitation on the exact simultaneous knowledge (measurement) of certain related physical phenomena (observables)."	58	"Solid knowledge of calculus and differential equations (including partial differential equations) and how these techniques are necessary to explain the theoretical underpinnings of physical phenomena."	25
W_D_294_A3	"energy, wave length, probability, momentum, quantization"	6	"complex numbers, operator, wave function, linear combination, eigenvalue"	8

CHAPTER 4: ANALYSIS & CONCLUSIONS

4.1: ANALYSIS. To probe physical chemistry experts' beliefs about the literature grounded dichotomy between conceptual and mathematical knowledge[1], participants of the FPPQMA were asked to provide their view on which knowledge domain best described a variety of concept inventory questions. The results of this study show evidence that physical chemistry experts selected knowledge domains best describing survey items with a moderate degree of consistency. Figures 3.8 and 3.9 from the Data and Results Section showed that the majority categorization of knowledge domain for all items besides number 2 was "Mostly Conceptual", accounting for 54% of knowledge domain assignments. It was anticipated that "Mostly Conceptual" should be the majority knowledge domain assignment as the concept inventory questions used in the FPPQMA came from concept inventories claiming to evaluate conceptual knowledge[6,4,12,7]. On the other side of this coin, it is interesting to note that approximately 42% of participant responses contained a mathematical component (~12% "Mostly Mathematical" and ~29% "Equally Conceptual and Mathematical"). It would be reasonable to assume that expert responses to questions lauded by developers as testing conceptual understanding might have selected the knowledge domain "Mostly Conceptual" more than ~50% of the time. From the physical chemistry education literature, we know educators believe there is a distinction between conceptual and mathematical knowledge[1], but what is it that differentiates these two knowledge domains? Before we respond to what these knowledge domains are believed to be by physical chemistry experts, let us take time to outline what our data suggest they are not.

The results of this study indicate that the distinction between mathematical and conceptual knowledge domains is not dependent on superficial features of question design, such as how information is represented or what type of subject matter is involved. Statistical analysis which controlled for these factors indicated there was no clear relationship between the knowledge domains selected by physical chemistry experts and the ACS topic best describing the survey items they were responding to. Nor was a clear relationship found between the type of representational form inherent to a survey item and the assignment of knowledge domain. These finding precipitate from the data shown in Tables 3.13-3.16. Previous studies in the general chemistry literature have demonstrated that chemistry experts, in general, categorize their knowledge based on deep structural features in lieu of surface features - like representational form – which are often relied on by novice chemists[35]. As such, it was assumed likely, and found ultimately true, that this trend would apply to experts of physical chemistry as well.

The FPPQMA survey data was also analyzed for the influence that a host of participant demographics had on expert knowledge domain assignments. Demographic analysis included examination of knowledge domain assignments for individual survey items as well as the average knowledge domain application per participant. This analysis revealed no discernable relationship between a subject's knowledge domain assignment and the US Region of their university, the highest degree offered by their institution, the Carnegie classification of their university, the research specialization of the participant, the last time the participant taught physical chemistry, nor how many times a participant had taught physical chemistry. Data supporting these conclusions are found in Tables 3.19-3.21. These findings support the conclusion that whatever it is physical chemistry educators believe about the dichotomy between conceptual and mathematical knowledge, their beliefs on the matter are relatively stable over geography and institutional character. To characterize what physical chemistry educators believed conceptual and mathematical knowledge were, a coding scheme was developed and applied to the qualitative portions of the FPPQMA survey data.

It was found that intuition was the most frequently applied code in our data. The code "Intuition" was applied to instances where a participant's response was general and/or undefined. For example, this representative quote from participant MW_D_326_Q1, "You understand the math needed to apply a concept for [an] application". Intuition was applied to the prompt "what is conceptual knowledge?" three times as often as it was applied to the prompt "What is a mathematical understanding?", as shown in Figure 3.5. We believe this to be, in part, because physical chemistry experts have fewer well-defined terms that describe what conceptual knowledge is, whereas they do have a shared vocabulary describing the mathematics relevant to physical chemistry. As such, participants are left to their own personal lexicon to capture the essence of conceptual understanding, thus leading to a higher frequency of general and non-specific responses. This claim is further substantiated by the average word counts of participant responses to our prompts, "What are the most important [concepts/mathematical tools] (up to 5), if any, for students to take away form an undergraduate physical chemistry course focused on quantum mechanics?". It was found that participants, on average, used 5.6 more words to describe concepts than they did to describe mathematical tools. These data were shown in Table 3.22. Additionally, the emergent epistemological codes "SynCon" and "SynMath", which capture synonyms representing conceptual and mathematical understanding, themselves show a similar imbalance. The code "SynCon" included three words deemed appropriate synonyms for concept: idea, qualitative, and principle, while "SynMath" only includes the term "quantitative." It seems an appropriate interpretation of these data to conclude physical chemists do not share a common language articulating what the conceptual knowledge domain is, while they do appear to share language describing the mathematical knowledge domain. These findings, though interesting, do not help describe what defines the distinction between the conceptual and mathematical knowledge domains. We are pleased to report here that our survey did yield results which may help make the distinction.

The dichotomous distribution of the codes "Unpaired" and "Paired" between the two prompts, "what is a conceptual understanding?" and "what is a mathematical understanding?", respectively, provided us with some clarity as to the distinction between the two knowledge domains. The code "Paired" was applied to participant responses indicating that concepts and mathematics were not necessarily distinct in physical chemistry (e.g., "The ability to make the mathematical manipulations necessary to complete problems of a conceptual nature." - NE_D_581_M5.), while the code "Unpaired" was used to capture responses showing clear reference to mathematical knowledge and conceptual knowledge being distinct domains (e.g., "…I think of conceptual explanations as being able to explain something in words without equations." - W_M_55_V6). It was found that the code "Paired" was applied to the prompt "what is a mathematical understanding" nearly twice as often as it was to the prompt "what is a conceptual understanding?". Similarly, unpaired was applied at nearly twice the rate favoring "what is a conceptual understanding." These results were shown in Table 3.5. To explain this result, we posit that it is possible physical chemistry experts believe the relationship between the conceptual and mathematical knowledge domains is *not* bi-directional; physical chemistry experts appear to believe that a student's mastery over mathematical knowledge must inherently include mastery of conceptual knowledge, but not the other way round. This idea is captured clearly in the response of participant MW_B_131_R10, who states, “Mathematical understanding is being able … to express a concept correctly using the language and tools of mathematical relationships…”. We believe these results provide a plausible explanation for the literature grounded discrepancy between physical chemistry educators’ goals for students to develop a conceptual understanding of physical chemistry despite their overreliance on mathematical assessment[1]. If mathematical knowledge is believed to inherently include - at least to some degree - conceptual knowledge, evaluation of a student’s mathematical comprehension could be thought of as evaluation of both knowledge domains, and thus the discrepancy may not be oversight on the part of physical chemistry educators, but rather evidence of their definitional understanding of the two knowledge domains. It is important to note here that the design of the FPPQMA emphasizes the dichotomy between the conceptual and mathematical knowledge domains. It is possible that by structing the survey as we did, we influenced participants to respond in a manner that supported the dichotomy between the two knowledge domains. This was noted by participant SE_B_13_L2, who stated, “Having both questions together like this seems to set the tone for a forced division between two forms of understanding.” And participant SE_D_178_W9 who stated, “Mathematical understanding … does not really exist.” Follow-up interviews with participants are necessary to evaluate if our findings are genuine or artifacts of the survey design.

It is also interesting to note that of 20 survey items, assessment item 2 was the only inventory question receiving “Mostly Mathematical” as the majority knowledge domain assignment. In the authors opinion, the notable difference between assessment item 2 and the rest of the survey items is the lack of application for the mathematics included in the question. Figure 4.1 shows assessment item 2.

Assessment Item 2

If you have three variables (r, θ, and ϕ) describing a wavefunction and the three variables do not depend on each other, then

A) the full wavefunction can be written as a sum of single variable functions.

B) *the full wavefunction can be written as a product of single variable functions.

C) the three variables should be transformed into variables that depend on one another.

D) the full wavefunction can be written as a linear combination of single variable functions.

Figure 4.1: Assessment Item 2. This figure shows assessment item 2 of the FPPQMA Survey. This was the only item of the 20 items evaluated that received a majority assignment of "Mostly Mathematical" as the most appropriate knowledge domain.

For all other questions in the survey, a case could be made that a relationship between the physical world and the mathematics used to describe it are inherent in the question. As such, most of the survey items could be solved by a student invoking relevant information from the associated systems. For example, in survey item 4 (shown in Figure 4.2), a student's realization that momentum, speed, and kinetic energy are all related terms could lead them to the correct answer without any knowledge of the uncertainty principle. Whereas assessment item 2 is unlikely to be answered by an undergraduate student of physical chemistry using any problem-solving strategy[34] *besides* recalling the mathematical formalisms of wave functions. This observation then suggests that not all mathematical questions are believed by physical chemistry experts to include a conceptual component. It should be noted this is the same logic which was previously put into question what it is that concept inventory questions are measuring (QCCI, item 10, shown in Figure 1.1).

Assessment Item 4

According to the uncertainty principle, the more we know about an electron's position, the less we know about its

A) speed.

B) momentum.

C) kinetic energy.

D) *all of these.

Figure 4.2: Assessment Item 4. This figure shows assessment item 4 from the FPPQMA. This question can be answered by a student's realization that momentum, speed, and kinetic energy are all related terms. No knowledge of the uncertainty principle is necessary.

We know from the relative distribution of the code SynMath (93%) and Symbols (94%) applied to the prompt "in your own words, what is a mathematical understanding?" that physical chemistry experts believe mathematical questions to be quantitative in nature and to include mathematical formalisms ("[Mathematical understanding] involves quantifying things with numbers and calculating specific answers for specific conditions in an experiment." - NE_D_581_M5). It appears, then, based on assessment item 2, that there is some limit to the implicit connect between conceptual and mathematical knowledge; at some point mathematical formalism simply becomes that. Where the line between questions of a purely mathematical nature and a blend of conceptual and mathematical knowledge is remains to be determined. In an attempt to better understand this distinction, participant knowledge domain assignments were converted to the values 1 = Mostly Mathematical, 0 = Equally Conceptual and Mathematical, and -1 = Mostly Conceptual, and averaged by question. This process yielded a singular value for each survey item describing the average knowledge domain selected which could be placed a continuum from Mostly Conceptual (-1) to Mostly Mathematical (+1), equally conceptual and mathematical being central between them (0). Figure 4.3 depicts this analysis. We found that 17 of 20 survey items were thought by participants to be more conceptual in nature than mathematical; however, items 2, 8, and 12 were found to be more mathematical in nature. Beyond our speculation into item number 2, this analysis does not provide rational for the observed difference in average knowledge domain application of these survey items. Follow-up interviews with participants to determine *why* certain items on the FPPQMA are thought to be more mathematical in nature will be an important contribution to the future work of this study.

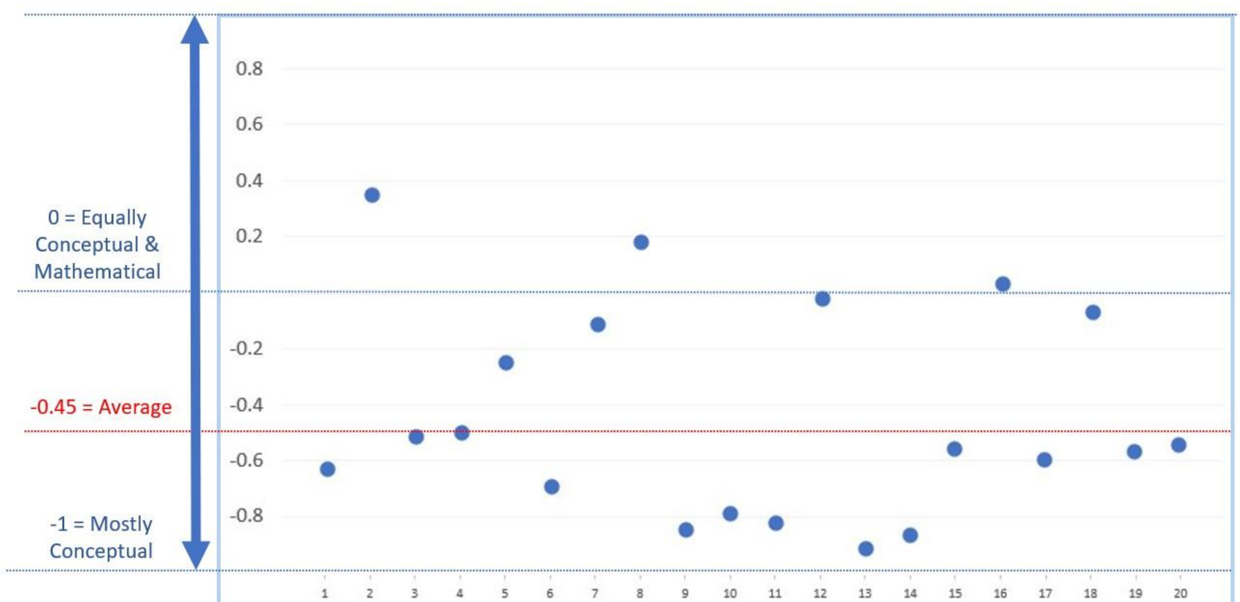

Figure 4.3: Knowledge Domain Assignents, Per Question, Continuum. These data depict the average knowledge domain assingments of all items on the FPPQMA. The domain assignemts were averaged, yeilding the values shown in the figure above. Items 2, 8, and 12 are thought by participants to be more mathematical in nature than the remaining survey items.

The last portion of our analysis pertains to the relationship between the assignment of the conceptual and mathematical knowledge domains to items in our survey, and the organization framework Technological-Social Dualism (TSD)[16]. In Technological-Social Dualism, different scientific tasks and practices are described as either *technical* - hard skills, often ascribed as masculine - or *social* - soft skills, often described as feminine (the authors of this thesis acknowledge the documented harms of these gender ascriptions and include them solely as a historical treatment of TSD[16]). If we return to the code distribution data reported in Table 3.7 (a replica of which is shown in Table 4.1, below) and view carefully the descriptions of codes therein, we find that the distribution of codes between the two knowledge domains approximately replicated the demarcations drawn by the TSD framework.

Table 4.1: Codes Grouped by Dominant Distribution between Categories. These data show the groups which our codes are were most often applied to. A codes placement in a category indicates it was applied to that domain more than 55% of the time. The "Evenly Distributed" bin was reserved for codes whose distributions were both between 45% and 55% in each domain.

Conceptual Leaning	Mathematical Leaning	Evenly Distributed
Intuition	Symbols	Relationships
SynCon	Algorithm	Predict
Explain	SynMath	Apply
Transfer	Problem	Error404
Unpaired	Tool	
Diagram	Interpret	
Word	Generate	
Describe	Paired	
Simplify	Modeling	
Teach		
Argument		
Memorization		

Codes which have some social aspect or a parameter which pertains to the transfer of information (Explain, Transfer, Diagram, Word, Describe, Teach, and Argument) are all predominately coded in response to the conceptual prompt. Conversely, codes which pertain directly to one's own understanding, and/or technical aspects like the tools and methods used to develop understanding and solve problems (Symbols, Algorithm, Problem, Tool, Interpret, Generate, and Modeling) are coded predominantly in response to the mathematical prompt. It seems that physical chemistry experts believe that conceptual knowledge is inherently more social in nature, as evidenced by this quote from participant SE_D_531_T8, "A criterion for conceptual understanding is whether you can explain the theory to your grandma. (No disrespect to Grandma.)". Mathematical knowledge, then, seems to be believed by physical chemistry experts to be more individualistic and technical in nature – it is more closely related to the tools and processes through which an individual learns quantum mechanics than it is one's ability to express that understanding. Participant SE_D_516_W3 is quoted as saying "[Mathematical understanding] is the understanding of the mathematical relationships that help us 1) learn about and 2) infer information from a specific subject".

4.2: LIMITATIONS. The statical analyses performed in this thesis are only a portion of those necessary to finalize this work. As noted in the data and results section, one-way ANOVA analysis followed by error adjusted iterative t-testing were used to draw conclusions about the relationship between various parameters of inventory items, personal research demographics, and the beliefs of physical chemistry experts regarding these inventory items. These statistics were performed under the assumption that these data are normally distributed. Further non-parametric testing and ANOVA post-hoc tests are necessary to ensure the validity of the claims included in this manuscript.

4.3: CONCLUSIONS. The results of the FPPQMA survey have provided insight into physical chemistry experts beliefs about the nature of conceptual and mathematical knowledge. Our study found evidence that experts consider the two knowledge domains distinct but intimately related, believing that conceptual understanding of quantum subjects presupposes mathematical understanding. For this reason, we suggest that the perceived overreliance of mathematical evaluation found in undergraduate physical chemistry courses[1,2] may, in fact, *not* be oversight on the part of physical chemistry educators, but rather indicative of experts' belief that evaluation of students' mathematical understanding simultaneously assesses their conceptual understanding of the subject at hand. Additionally, the results of our study suggest that physical chemistry experts lack a shared vocabulary describing what conceptual understanding *is.* It is possible this lack of specificity in definitional terms is cause for the noted inadequacies of efforts to articulate the essence of conceptual understanding/knowledge[1,27]. Last, this study found that physical chemistry experts differentiate conceptual and mathematical knowledge (and skills generally associated with each domain) along lines nearly identical to those drawn by the Technological-Social Dualism Framework; experts believe that conceptual knowledge is generally more social in nature, while mathematical knowledge is inherently more technical.

In response to these findings, the authors of this study recommend educators of quantum chemistry desiring that their students develop a conceptual understanding take time to reflect deeply on their own interpretation of this target goal. Is conceptual understanding simply being used as a synonym for "understanding beyond memorization"? If so, are there more tangible learning targets which might help students meet this end? Further, how do educators intend to evaluate students' conceptual understanding? Are calculations to be considered evidence that students are, in fact, meeting the desired goal? What social elements are integrated into physical chemistry course materials which might assist in the development of students' conceptual understanding? Are students being given opportunities to teach and share with others? Are they being given opportunities to use varying symbolic nomenclature that doesn't rely heavily on mathematical formalism? Are students being encouraged to distill and paraphrase complex ideas?

As this thesis and prior studies have demonstrated, pinpointing what conceptual understanding *is* and how one evaluates it is no trivial task. Given the widely varying interpretations of the term, it well may be the case that no formal definition of conceptual understanding will ever be satisfactory. As such, the responsibility for the appropriate application and assessment of the term (when used as a learning target) becomes the responsibility of each individual physical chemistry educator.

4.3: FUTURE WORK. Future work and suggested direction for the continuation of this study are as follows (presented in approximate order of how these ideas appear in this thesis):

- Perform analysis of prompts included in the FPPQMA pertaining to the depth of knowledge students must have to perform tasks (Answer the question and explain the question) related to the survey items. This data, in conjunction with knowledge domain assignment, and ACS-topic/representational form descriptors, will help elucidate how physical chemistry experts believe students apply their understanding of the knowledge domains to questions of varying content and representation.
- The analysis provided in this thesis views the codes capturing physical chemistry experts' beliefs about the two proposed knowledge domains individually and globally (i.e., how does one specific coded or a group of codes appear to be distributed thought out the data). This did reveal some very interesting trends, but further analysis to determine how frequently codes are applied together, as pairs or small groups, would provide a greater understanding of how physical chemistry experts define the two proposed knowledge domains.
- Finer grain analysis of the impact that ACS topic and representational form have on the knowledge domain sections of experts should be included. The analysis in this thesis suggests that globally there is no meaningful correlation between these parameters and the assignment of knowledge domain, but there does exist evidence in our data that influence is still possible. Take for example the data shown in Figure 4.4 which show three survey items (items 2, 5, and 14), all represented differently but relating most directly to the ACS topic Postulates of Quantum Mechanics. As can be seen in Figure 4.4, the textual

question (item 14) shows a much higher assignment of "Mostly Conceptual" than does the symbolic question (item 2), which shows a higher response of "Mostly Mathematical." As noted in this thesis, it does appear to be the case that the correlation between form, topic, and knowledge domain disappears when looking at the data globally, but these data indicate some relationship still exists.

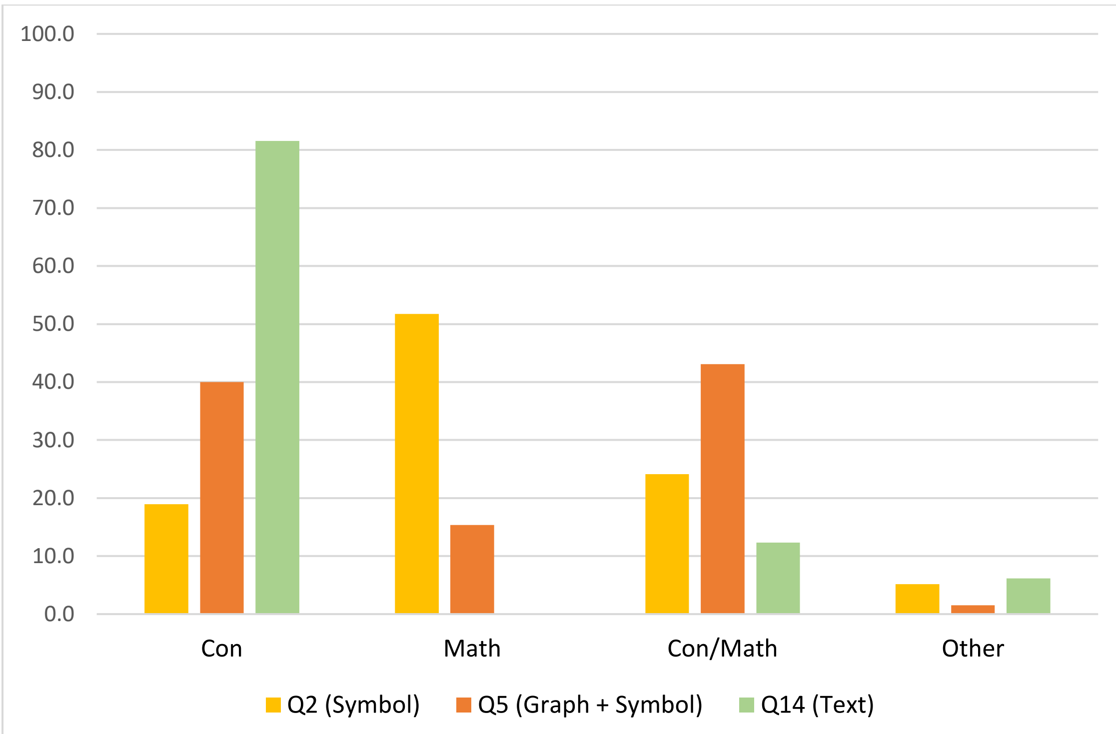

Figure 4.4: Local Example of Relationship Between Form and Knowledge Domain Assignments.

- Further analysis is needed to determine why some of the survey items were determined by experts to be more mathematical than conceptual in nature (Items 2, 8, 12). Our statical analyses indicate experts interact with these items differently than the others, but not why. Follow-up interviews with participants would be the preferable method of analysis.
- Perform non-parametric and post-hoc ANOVA analysis on data pertaining to expert knowledge domain assignments to increase the robustness of our findings

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SUPPLIMENTAL

S.1: FPPQMA SURVEY ITEMS

Assessment Item Sources:

Assessment Item 1 Used in the FPPQMS. Source: QPCS

Assessment Item 2 Used in the FPPQMS. Source: QCCI

Assessment Item 3 Used in the FPPQMS. Source: QMCS

Assessment Item 4 Used in the FPPQMS. Source: QPCS

Assessment Item 5 Used in the FPPQMS. Source: QMCS

Assessment Item 6 Used in the FPPQMS. Source: QCCI

Assessment Item 7 Used in the FPPQMS. Source: QPCS

Assessment Item 8 Used in the FPPQMS. Source: QMCA

Assessment Item 9 Used in the FPPQMS. Source: QMCA

Assessment Item 10 Used in the FPPQMS. Source: QMCS

Assessment Item 11 Used in the FPPQMS. Source: QPCS

Assessment Item 12 Used in the FPPQMS. Source: QPCS

Assessment Item 13 Used in the FPPQMS. Source: QMCS

Assessment Item 14 Used in the FPPQMS. Source: QCCI

Assessment Item 15 Used in the FPPQMS. Source: QCCI

Assessment Item 16 Used in the FPPQMS. Source: QMCA

Assessment Item 17 Used in the FPPQMS. Source: QCCI

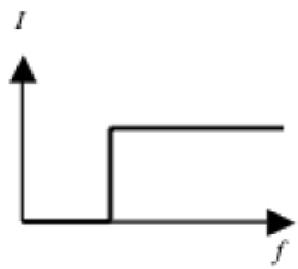
Assessment Item 18 Used in the FPPQMS. Source: QMCS

Assessment Item 19 Used in the FPPQMS. Source: QPCS

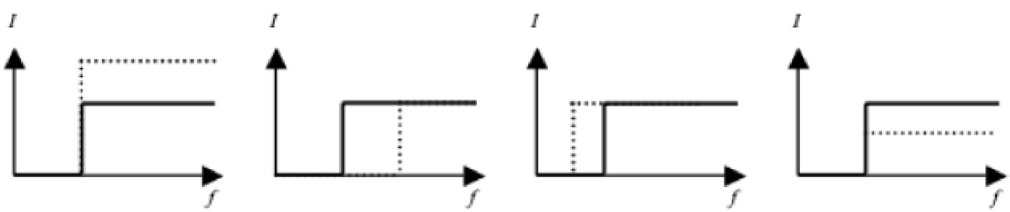
Assessment Item 20 Used in the FPPQMS. Source: QMCA

Assessment Item 1

In a hypothetical experiment to demonstrate the photoelectric effect, a light source of variable frequency is shone on a photo-sensitive surface. Ejected photoelectrons are collected by an anode. A graph of the resulting photocurrent (I) as a function of frequency (f) looks like this.



Which graph would be most appropriate when the work function of the surface is increased?



A. *B. C. D.

Assessment Item 2

If you have three variables (r, θ, and ϕ) describing a wavefunction and the three variables do not depend on each other, then

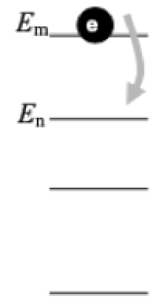
A) the full wavefunction can be written as a sum of single variable functions.

B) *the full wavefunction can be written as a product of single variable functions.

C) the three variables should be transformed into variables that depend on one another.

D) the full wavefunction can be written as a linear combination of single variable functions.

Assessment Item 3



The diagram at the right shows the electronic energy levels in an atom with an electron at energy level E_m. When this electron moves from energy level E_m to E_n, light is emitted. The greater the energy difference between the electronic energy levels E_m and E_n...

A) ... the more photons emitted.

B) ... the brighter (higher intensity) the light emitted.

C) ... the longer the wavelength (the more red) of the light emitted.

D) *... the shorter the wavelength (the more blue) of the light emitted.

E) More than one of the above answers is correct.

Assessment Item 4

According to the uncertainty principle, the more we know about an electron's position, the less we know about its

A) speed.

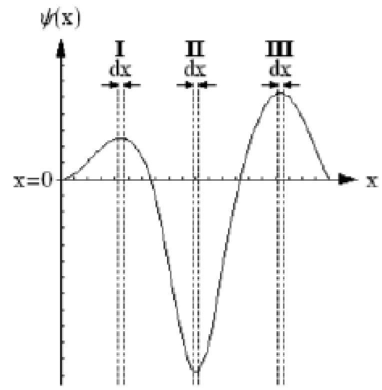
B) momentum.

C) kinetic energy.

D) *all of these.

Assessment Item 5

The plot at the right shows a snapshot of the spatial part of a one-dimensional wave function for a particle, $\psi(x)$, versus x. $\psi(x)$ is purely real. The labels I, II, and III indicate regions in which measurements of the position of the particle can be made. Order the probabilities, P, of finding the particle in regions I, II, and III from biggest to smallest.



A) $P(\text{III}) > P(\text{I}) > P(\text{II})$

B) $P(\text{II}) > P(\text{I}) > P(\text{III})$

C) $P(\text{II}) > P(\text{I}) > P(\text{III})$

D) $P(\text{I}) > P(\text{II}) > P(\text{III})$

E) *$P(\text{II}) > P(\text{III}) > P(\text{I})$

Assessment Item 6

How is the harmonic oscillator model in quantum mechanics (QM) analogous to the motion of a classical mechanics (CM) spring?

A) The wavefunction oscillates in time like a spring.

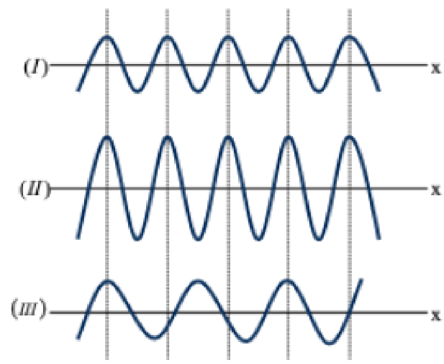
B) The motion of the harmonic oscillator slowly damps until motion has stopped.

C) The QM wavefunction has oscillating momentum much like the CM spring.

D) *The classical limit of the QM harmonic oscillator, for the most probable location, yields the CM spring results.

Assessment Item 7

Three particles of equal mass are traveling in the same direction. The de Broglie waves of the three particles are as shown.



Rank the speeds of the particles (I), (II), and (III) by choosing one of these four possibilities.

A) $v_{II} > v_I > v_{III}$

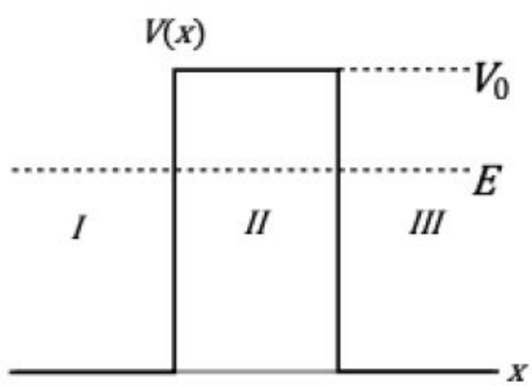
B) $v_{II} > v_{III} > v_I$

C) $*v_I = v_{II} > v_{III}$

D) $v_{II} > v_I = v_{III}$

Assessment Item 8

Suppose a particle of mass m and total energy E has a potential energy function, $V(x)$, shown below. Note that in the region II, $E < V_0$.



What is the general solution to the time independent 1-D Schrodinger equation in region II? Assume k is a positive real number.

A) $Ae^{ikx} + Be^{-ikx}$

B) $*Ae^{kx} + Be^{-kx}$

C) Ae^{-ikx}

D) Ae^{-kx}

Assessment Item 9

Consider a system where we can measure two quantum mechanical observables, "color" (represented by the $\hat{C}$ operator) and "size" (represented by the $\hat{S}$ operator). The "color" operator has three eigenvalues (red, green, and blue) and three corresponding eigenstates ($|r\rangle$, $|g\rangle$, and $|b\rangle$). The "size" operator also has three eigenvalues (small, medium, and large) with three corresponding eigenstates ($|s\rangle$, $|m\rangle$, and $|l\rangle$).

We wish to understand how color and size interact. Since we cannot see the "color" or "size" of our particles with our eyes, we build a lab with a ColorTron^{TM} device which measures the "color" eigenvalue of a particle and a SizeUp^{TM} device which measures the particle's "size" eigenvalue.

In the setup just described, an experimenter measures the color of the particles and then **immediately** runs all particles which measured red through the ColorTron^{TM}. What are the possible values of this second measurement?

A) *The only possible measurement is red with a 100% probability of measurement.

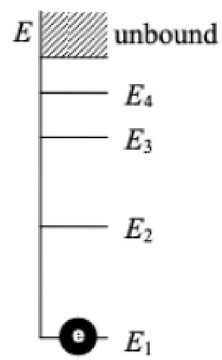
B) Red, green, and blue can be measured with equal probabilities.

C) Red, green, and blue can be measured, but their associated probabilities of measurement cannot be determined from the information given.

D) There is not enough information to answer this question.

Assessment Item 10

An electron in an atom has the energy level diagram at the right. The electron is in its lowest energy state, as shown in the diagram. What is the lowest energy photon that it can absorb?



A) E_1

B) E_2

C) *$E_2 - E_1$

D) $E_4 - E_3$

Assessment Item 11

In an experiment to demonstrate the photoelectric effect the following observations are made:

- light of high frequency shone onto some materials causes electrons to be ejected, and
- if the frequency of light is decreased (with any amplitude) there is a cut-off frequency below which electrons are no longer ejected

These observations are believed to support a particle theory of light, rather than a wave theory. Which one of these statements is inconsistent with the observations?

A) In a particle theory, ejection of electrons is explained by collisions with photons. Each collision can give a single electron enough energy to escape.

B) In a wave theory, ejection of electrons is explained by the electromagnetic wave causing the electrons to vibrate, which gives some electrons enough energy to escape.

C) In a particle theory, the cut-off is explained because at very low frequencies the photons have very low energies and no individual photon has enough energy to eject an electron.

D) *In a wave theory, the cut-off is explained because a very low frequency wave could not make the electrons vibrate energetically enough, even at very high amplitudes.

Assessment Item 12

What will happen when a positively charged particle is moving through an <u>electric</u> field, in the same direction as the field, and is therefore speeding up?

A) The de Broglie wavelength of the particle will increase.

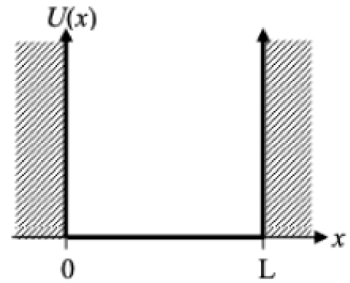
B) *The de Broglie wavelength of the particle will decrease.

C) The de Broglie wavelength of the particle will remain the same.

Assessment Item 13

QMCS 6. Consider an electron with the potential energy

$$U(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x < 0 \text{ or } x > L \end{cases}$$



This potential energy function, plotted at the right, is often referred to as an infinite square well or a rigid box. Your electron is in the lowest energy state of this potential energy, with a wave function $\psi(x) = \psi_1(x)$ and a corresponding energy E_1. Suppose you first measure the position of this electron very precisely, without destroying the electron. After measuring the position, you measure the energy of the same electron. Which of the following statements describes the result of this energy measurement?

A) The value that you measure will be E_1.

B) *The value that you measure could possibly be E_1.

C) The value that you measure will *not* be E_1.

Assessment Item 14

In quantum mechanics, electrons in atoms are described by a wavefunction. What do wavefunctions describe about the system?

A) The average position of electrons over time.

B) *Once squared, the probability of finding an electron.

C) The combination of all pathways the electrons can take to orbit the nucleus.

D) The amplitude of the vibrations that electrons make as they move around the nucleus.

Assessment Item 15

Consider the solutions to the one dimensional "particle in a box" model. How does the quantum mechanical solution change for a particle contained within a zero potential energy, fixed length "box" surrounded by an infinite potential versus the same particle surrounded by a finite potential?

A) The solutions are the same because the length of the "box" is fixed.

B) The gaps between energy levels decrease in the solution of the infinite potential as compared to the finite potential box.

C) *The solutions differ in that the finite potential allows tunneling while the infinite potential does not.

D) The solution to the finite potential can be solved analytically, while the infinite potential solution cannot be, thus approximations must be used.

Assessment Item 16

Consider a system where we can measure two quantum mechanical observables, "color" (represented by the $\hat{C}$ operator) and "size" (represented by the $\hat{S}$ operator). The "color" operator has three eigenvalues (red, green, and blue) and three corresponding eigenstates ($|r\rangle$, $|g\rangle$, and $|b\rangle$). The "size" operator also has three eigenvalues (small, medium, and large) with three corresponding eigenstates ($|s\rangle$, $|m\rangle$, and $|l\rangle$).

We wish to understand how color and size interact. Since we cannot see the "color" or "size" of our particles with our eyes, we build a lab with a ColorTron^{TM} device which measures the "color" eigenvalue of a particle and a SizeUp^{TM} device which measures the particle's "size" eigenvalue.

In the setup just described, 1000 red particles are immediately run through the SizeUp which measures the small eigenvalue 200 times, the medium eigenvalue 300 times, and the large eigenvalue 500 times. Which one of the following could be a valid representation of the $|r\rangle$ state in the "size" basis?

A) $200\,|s\rangle + 300\,|m\rangle + 500\,|l\rangle$

B) $\frac{1}{10}(2\,|s\rangle + 3\,|m\rangle + 5\,|l\rangle)$

C) *$\frac{1}{\sqrt{10}}(e^{i\alpha_1}\sqrt{2}\,|s\rangle + e^{i\alpha_2}\sqrt{3}\,|m\rangle + e^{i\alpha_3}\sqrt{5}\,|l\rangle)$

D) $\frac{1}{10}e^{i\alpha}(\sqrt{2}\,|s\rangle + \sqrt{3}\,|m\rangle + \sqrt{5}\,|l\rangle)$

E) None of the above.

Assessment Item 17

What is a major effect of anharmonicity on the vibrational energy?

A) The ground state vibrational energy increases in energy.

B) The ground state vibrational energy decreases in energy.

C) The difference between vibrational energy levels increases.

D) *The difference between vibrational energy levels decreases.

Assessment Item 18

You see an electron and a neutron moving by you at the same speed. How do their wavelengths λ compare?

A) $\lambda_{neutron} > \lambda_{electron}$

B) *$\lambda_{neutron} < \lambda_{electron}$

C) $\lambda_{neutron} = \lambda_{electron}$

Assessment Item 19

The Heisenberg Uncertainty Principle is mostly applied to very small objects such as electrons and protons. Why don't we use the uncertainty relation on larger objects such as cars and tennis balls?

A) The errors of measurement can always, in principle, be made smaller by using more sensitive equipment.

B) Large objects at any instant in time have an exact position and momentum and with sufficient care we can measure both precisely.

C) Large objects obey Newton's laws of motion, to which the uncertainty principle does not apply.

D) *Because it does apply to large objects, but the uncertainties are so small that we don't notice them.

Assessment Item 20

Consider a spin-1 particle sitting in a uniform magnetic field oriented in the +z direction. The Hamiltonian for this particle is proportion to S_z (the z-component of spin). The normalized eigenstates of S_2 for this particle are labeled as $|-1\rangle$, $|0\rangle$, and $|1\rangle$, with corresponding eigenvalues $-\hbar$, 0, and $+\hbar$.

A particle starts in a quantum state given by $|\psi\rangle = \sqrt{\frac{4}{5}}|-1\rangle + \sqrt{\frac{1}{5}}|1\rangle$.

Suppose you make a measurement of S_x (the x-component of spin).

Immediately after this measurement, you then measure S_z (the z-component of spin). At this point, what value(s) could you get for the z-component of spin of the particle?

A) $\frac{4}{5}(-\hbar) + \frac{1}{5}(+\hbar)$

B) $-\hbar$ only

C) Just $-\hbar$ or $+\hbar$

D) *$+\hbar$, 0, or $-\hbar$

E) Any continuous angular momentum value between $-\hbar$ and $+\hbar$.

S.2: CODEBOOK (DEFINITON & EXAMPLES)

Problem - Reference to solving problems (in the affirmative). Reference to an academic problem (e.g., test, quiz, homework, or reference to "solving for a variable, value, or answer") to which an idea may be applied.

Examples:
"Conceptual understanding is the type of understanding that allows a student to figure out how to solve a problem that they have never seen before." - NE_D_439_S3

"Understanding the concept and being able to problem-solve or derive a solution to a related topic." - MW_B_682_R2

Symbols – Reference to mathematical literacy (e.g., knowledge of symbols, formulae, and mathematical operations), or mention of mathematical components (e.g., variables, equations, techniques, etc.), operations, or symbols.

Examples:
"Being able to manipulate the equations to calculate useful information" - W_D_470_I3
"The ability to relate variables in a model to the whole." - NE_B_282_U1

Diagrams - Reference to images, diagrams, graphs, pictures, and non-equation/non-verbal mathematical representations.

Examples:
"Understanding in terms of a pictorial model" - W_D_294_A3
"There are many approaches to conventual understanding: pictorial description of a theory is one of them." SE_D_531_T8

Word - Reference to using written or spoken words to depict ideas and/or to convey understanding.

Examples:
"Ability to describe/explain features of a physical system or phenomenon in words …" SE_D_642_T10
"The ability to put into words the principles they learned." NE_B_442_C3

Explain - References to demonstrating one's knowledge and/or understanding by telling how/why something is true or occurs, which may include describing "cause and effect", using mathematical tools, or non-specific use of the word "explain". (Note: references to explaining to another person will be coded as "Teach").

Examples:

"The ability to express in plain (rather than 'scientific') language the cause and effects leading to a specific observation." - SW_D_408_W5
"Conceptual understanding is the ability to (1) explain a concept to others …" MW_B_131_R10

Teach - Reference to being able to share/communicate one's knowledge with another (not teacher).

Examples:
"An individual understands a concept when they can explain it to others … " - SE_D_502_T2
"A person has conceptual understanding of a mechanism or a process if he/she can explain this mechanism/process to an uninitiated person." - NE_B_70_W9

Modeling - Reference to models or modeling, using models in an expert-like way, and/or to mathematics being used for modeling.

Examples:
"A demonstrated ability to use mathematical tools to quantify the properties of a physical/chemical process. Typically this involves the direct application of models discussed in the classroom/lab." - MW_B_9_F6
"Being able to describe something with appropriate physical models …" - NE_B_601_V6

Argument – Reference to the justification of claims using scientific ideas and/or evidence to another.

Examples:
"Mathematical understanding refers to the ability for students to use math to precisely predict expectations for experiments and to defend a hypothesis derived from first principles." - NE_M_641_O5

"The ability to explain phenomena and justify theories and justify theories without mathematical derivations." – MW_D_327_Z10

Interpret - References to being able to make meaning from results and/or data.

Examples:
"Conceptual understanding refers to understanding how topics relate to each other and can be combined to interpret qualitative physical behaviors and experimentally observed trends." - NE_M_641_O5
"In contexts beyond mathematics itself, a person has mathematical understanding when they can explain how mathematics is used to interpret or predict behavior of a system." - SE_D_502_T2

Simplify – Reference to distillation of complex ideas to their essence, e.g, using simple, plain, or concise language to depict ideas. (Note: non-specific references to "basic" or "fundamental" concepts are coded as intuition).

Examples:

“Having an ability to comprehend and explain a phenomenon in lay terms.” MW_D_577_R8
“Using math as an efficient metaphor to summarize concepts and principles.” - W_D_49_Z4

Describe- Reference to using one's "own words" to describe ideas. References to describing ideas, including the use of the word describe.

Examples:
“Understanding the underlying chemistry in a way that you are rephrase the concept in your own words.” - row11con
“...to explain a system in such a way that your words create a picture in another person’s mind.” - 163con

Predict – References to making an inference about what a result should be.

Examples:
“...Being able to interpret an equation to predict trends or behaviors.” - W_B_592_T8
“The ability to describe a phenomenon using a theoretical model at a level that allows you to use the model to make predictions about new scenarios.” - SW_B_591_R6

Algorithm - References to being able to perform, solve, or compute mathematical calculations, operations, and derivation.

Examples:
“Being able to manipulate the mathematical algorithms necessary to solve a problem.” - SE_M_109_T4
“…[c]an manipulate mathematical theories, do calculations, etc.” - SW_D_467_Y3

Relationships - References to relationships between physical chemistry tools (models/math) and their applications, different modes of thinking (e.g., connection between different knowledge domains), or variables in an equation; knowing how concepts are connected to each other; having a mental (or visible) concept map / theoretical framework.

Examples:
“Understanding the qualitative relationships between parameters in a physical system in a way that can be applied to multiple scenarios, including ones not encountered before.” - NE_B_11_H8
“Understanding the physical relationships at a quantitative level …” - NE_D_223_L8

Intuition - References to understanding, intuition, perception or comprehension of ideas, concepts, or tools necessary for physical chemistry in non-specific ways. Unspecific uses of the words “basic” and “fundamental” are to be coded as intuition.

Examples:
“Students are expected to understand the basic ideas, for example of quantum mechanics.” - SE_D_462_E3

“[K]now the concept of a phenomenon and can describe it's physical meaning” - NE_D_374_L2

Apply - References to the application of a concept, theory, or idea, to a physical system. Physical systems include references to chemical systems, experiments, and synonyms like phenomenon and observation. (Note: the verbs "explain" and "describe" are not example of apply).

Examples:
"Knowledge of an idea or theory well enough to be able to apply the idea to a physical system." - MW_B_682_R2
"Being able to correctly apply quantitative symbolic formulas describing a phenomenon in a predictive manner." NE_D_485_K1

Generate - References to the generation of a model (e.g, mathematizing a physical system) based on observation or knowledge of the system.

Examples:
"The ability to express in equations the set of relationships between observations predicted by a theory." SW_D_408_W5
"Mathematical understanding refers to the ability for students to use math to precisely predict expectations for experiments and to defend a hypothesis derived from first principals." NE_M_641_O5

Transfer - References to use of quantum mechanical ideas in a new context, adjacent scientific field, or the "real world" (e.g., climate change, industrial applications, etc.)

Examples:
"… [t]aking the equations from above and integrating other concepts, and expanding the equation for a new s[c]enario …" W_B_592_T8
"Conceptual understanding is the type of understanding that allows a student to figure out how to solve a problem that they have never seen before." NE_D_439_S3

SynCon – Use of synonyms for concept, including "idea", "qualitative", and "principle".

Examples:
"Understanding qualitative relationships between parameters in a physical system in a way that can be applied to multiple scenarios ..." NE_B_11_H8
"Understanding the concepts and principals [*sic*] and being able to apply then [*sic*] to problems without resorting to canned processes." W_D_49_Z4

Memorization – Reference to understanding *not* being memorized or algorithmic.

Examples:
"Conceptual understanding is the type of understanding that allows a student to figure out how to solve a problem that they have never seen before. It is distinct from wrote [*sic*] memorization." - NE_D_439_S3
"Being able to solve mathematical problems mechanically, without conceptual understanding, would not meet the standard of mathematical understanding." - SE_D_502_T2

Paired - References to conceptual knowledge and mathematical knowledge not necessarily being distinct domains in physical chemistry.

> Examples:
> "… Ability to explain the mathematical relationships from a conceptual perspective is an important piece of true mathematical understanding of physical concepts." - NE_D_223_L8
> "Mathematical understanding presupposes conceptual understanding." - SE_D_502_T2

Unpaired - References to conceptual knowledge and mathematical knowledge being distinct domains in physical chemistry.

> Examples:
> "Conceptual understanding entails familiarity and knowledge (not necessarily detailed) of a larger view of a particular issue. As such, conceptual understanding extends to many facets, including those that do not require explanation via mathematics." - W_D_497_U1
> "Mathematical understanding is being able to follow mathematical rules and equations to derive the governing rules of physical phenomena. Mathematical understanding does not always lead to conceptual understanding." - SE_D_135_D2

Tool - Reference to mathematics being a tool used to perform functions related to physical chemistry.

> Examples:
> "An ability to articulate and understand the physical/chemical reasons for a calculated outcome or experimentally observed phenomenon. This can be demonstrated without the use of mathematical tools, and may benefit from drawn pictures and diagrams. - MW_B_9_F6
> "Math is a tool used to understand things." - NE_B_11_H8

SynMath - Use of "quantitative" as a synonym for mathematical.

> Examples:
> "Knowledge of common symbols representing numbers and concepts; specific methods of manipulating them in physical chemistry. This also includes interpretation of quantitive (sic) information such as reading information from graphs." - MW_D_527_W5
>
> "The ability to make accurate quantitative predictions about new chemical situations by citing the theoretical framework that is physical chemistry ideas." SE_M_665_O3

Error404 - Respondent stated they chose not to answer the question, acknowledged they had no definition, provided a circular response, or a response which did not correlate to the question prompt.

> Examples:
> "I choose not to answer this question." - NE_B_216_O5
>
> "Same as above" - W_D_495_P10

S.3: FLEISS KAPPA CALCULATION

Fleiss K

①

	math M	math E	math T
1	0	1	1
2	1	1	1
3	0	0	0
4	0	0	0
5	1	1	1
6	1	1	1
7	1	1	1
8	0	0	0
9	1	1	1
10	1	1	1
11	0	0	0
12	0	0	0
13	0	0	0
14	1	1	1
15	0	0	0
16	0	0	0
17	0	0	0
18	0	0	0
19	0	0	0
20	0	0	0

② ④

Subjects	Did not code	Did code	P_i
1	1	2	0.333333
2	0	3	1
3	3	0	1
4	3	0	1
5	0	3	1
6	0	3	1
7	0	3	1
8	3	0	1
9	0	3	1
10	0	3	1
11	3	0	1
12	3	0	1
13	3	0	1
14	0	3	1
15	3	0	1
16	3	0	1
17	3	0	1
18	3	0	1
19	3	0	1
20	3	0	1
P_j ③	0.61667	0.383333	P ⑤ 0.966667

⑥ P_e 0.527222

① Begin with binary data (1 = used code, 0 = did not)

② Create **a frequency table** using data from ①

③ Calculate the **proportion of codes assigned (P_j)** by, for each column:

- Σ entries / Nn
- N = number of subjects. n= number of coders
- Example: Σ column / (20 x 3) = 0.61
- *Interpret this as "how often a code was applied"*

④ Create a **Proportion of Agreement column (P_i)** by, for each row in the frequency table:

- Σ (sum of squares) – Σ entries / n(n-1)
- n=number of coders
- $(1^2 + 2^2) – (1+2) / 3(3-1) = 1/3$
- *Interpret these values as "the percentage of possible coincidences that were paired"*

⑤ Σ P_i column = **P**

- *Interpret this as "the percent of <u>total</u> coincidences that were paired"*

⑥ Σ sum of squares of P_j row **(P_e)**

- Interpret this as "the percent these observations occurred by chance"

⑦

$K = A_l + A_c / 1 – A_c$

Perform the calculation: **$K = (P-P_e) / (1-P_e)$**

(0.966667-0.527222) / (1-0.527222) = 0.929

Calculated using SPSS: 0.929

Use same Kappa statistic scale

S.4: CODING SCHEME DATA

Participant	Conceptual codes					
SE_D_135_D2	Intuition	syncon				
W_D_497_U1	Intuition	unpaired				
W_D_294_A3	diagram	modeling				
NE_D_223_L8	Relationships	diagram	apply	syncon		
MW_B_9_F6	Tool	diagram	explain	unpaired	apply	
MW_B_238_M5						
W_D_470_I3	Syncon	intuition	symbols	relationships		
MW_B_363_M7	Explain	word	diagram			
NE_B_282_U1	Apply	explain	intuition			
MW_D_465_O3	Describe	word	intuition			
MW_B_682_R2	Intuition	apply				
SW_D_408_W5	Simplify	word	apply	explain		
W_D_495_P10	Transfer	problem	intuition			
NE_B_442_E5	Simplify	word	intuition			
W_M_62_N4	Explain					
NE_M_641_O5	Syncon	relationships	interpret	apply		
NE_D_439_S3	Problem	memorization	transfer			
MW_D_331_T10	Apply	intuition				
SE_D_502_T2	Explain	teach	transfer			
MW_D_625_Y3						
NE_B_11_H8	Transfer	apply	syncon	relationships		
MW_D_527_W5	problem	modeling	intuition			
MW_D_327_Z10	explain	argument	unpaired			
NE_D_485_O5	apply	intuition	transfer			
W_B_592_T8	intuition	unpaired	problem	symbols	predict	
W_D_112_P6	intuition	apply	transfer			
W_D_49_Z4	memorization	intuition	problem	syncon		
NE_B_147_S7	intuition	relationships	explain			
NE_B_70_W9	explain	teach				
NE_B_601_V6	modeling	relationships				
SE_B_352_P4	intuition	unpaired				
NE_D_581_O7	paired	symbols	apply	predict	explain	syncon
SE_M_665_O3	apply	syncon	predict	transfer		
NE_M_93_E3	diagram	intuition	syncon			
SW_B_591_R6	predict	transfer	modeling			
MW_B_416_M1	word	diagram	unpaired	relationships		
NE_D_121_V8	transfer	syncon	intuition	problem		
MW_D_625_Q5	intuition	diagram	word			
SE_B_621_S1	syncon	unpaired	predict	explain		
NE_B_250_D2	modeling	apply	problem	predict		
SE_D_517_M9	intuition					
NE_D_581_M5	intuition	memorization	syncon			
MW_D_542_T10	Transfer	SynCon				
MW_B_122_C5	Intuition	SynCon				
SE_B_13_P6	Intuition	SynCon				
SE_D_151_Y3	Explain					
SE_D_548_O7	Relationships	Problem	Transfer			
NE_B_377_T10	Intuition	Relationships				
SE_B_569_Q1	Intuition	Relationships	Symbols	Paired		
SE_B_149_V10	Predict	Paired	SynCon	intuition		
W_B_166_L2	Intuition	SynCon				
W_B_592_V10	Intuition	Relationships	Word	Diagram	Explain	
MW_D_528_B10	Explain	Teach	Word			
MW_D_78_D6	Relationships	Problem	SynCon	intuition		
SE_D_502_Q9	Explain	SynCon	Paired	Relationships		
MW_D_577_D10	Intuition	SynCon				
MW_M_407_V4	Explain	Predict	modeling			
NE_D_347_V4	SynCon	Unpaired				
MW_B_627_E9	SynCon	Apply	Intuition	Paired	modeling	
NE_B_6_E5	SynCon	Intuition	Relationships			
NE_D_341_X10	Paired					
NE_D_581_K3	Explain	Word	Diagram	Symbols	Paired	
NE_D_485_K1	Intuition					
NE_B_649_Q3	Intuition	Error404				
W_D_49_X2						
W_D_633_N8	Problem	Intuition				
W_M_55_V6	Explain	Apply	Relationships	Unpaired	SynCon	
NE_B_70_K7	Transfer					
MW_M_679_N8	Predict	Intuition				
NE_B_399_H10	Intuition					
SW_D_467_V10	SynCon	Apply	Unpaired			
NE_D_614_A7	Intuition	Transfer				
W_M_205_G1	Intuition	Relationships	Apply			
W_D_470_P10	SynCon	Relationships	Intuition			
MW_B_669_A5	Paired	SynCon	Word	Diagram		
W_D_496_B2	SynCon	Intuition				
NE_D_512_D4	Transfer	SynCon				
NE_B_677_J4	SynCon	Relationships	Intuition			

SW_D_608_O5	SynCon	intuition				
NE_B_179_E7	Intuition	Predict	Apply			
MW_M_576_H8	SynCon	Unpaired	Predict	Explain	Apply	
SE_B_569_R2	SynCon	Problem	Intuition			
SE_B_354_Q5	Explain	SynCon	intuition			
MW_M_546_E7						
NE_B_263_P4	Intuition	Relationships	SynCon			
NE_D_537_H8	Intuition	modeling				
NE_B_399_I1	Paired	Teach				
MW_D_577_R8	Explain	Simplify				
NE_M_93_Z8	Error404					
SE_D_100_N2	Relationships	Explain	Transfer	Paired		
SE_D_647_M9	Intuition	SynCon				
NE_B_634_O9	Intuition	SynCon				
NE_D_535_S3	Teach	Simplify	Explain			
NE_D_486_Q7	Intuition	Unpaired				
SW_M_386_D10	Relationships	Intuition	modeling			
MW_D_549_W5	Intuition	SynCon				
MW_D_278_I9	Intuition	Symbols				
NE_D_51_G1	word	Intuition				
MW_B_127_I1	Relationships	Intuition				
W_B_339_K7	Modeling	word	Paired			
MW_D_666_R6	Intuition	SynMath				
SW_D_466_R6	SynMath					
SE_B_221_F2	Apply	Problem				
SE_B_572_Z10	Relationships	Paired	Modeling	Symbols		
NE_B_651_T6	Relationships	SynCon				
W_M_60_F6	SynCon	Explain				
NE_D_341_T6	Intuition					
W_B_592_S7	Intuition					
MW_B_148_T8	Intuition	SynCon	Apply	Modeling		
W_D_470_L6	word	Diagram	Relationships	Simplify		
SE_D_462_E3	SynCon	Problem	intuition			
SW_D_520_U7	word	Describe				
MW_D_78_A3						
SE_D_288_Z6	SynCon	Explain	Unpaired			
NE_D_92_W5	Explain	Syncon	diagram	predict	modeling	
MW_B_261_O3	intuition	syncon				
SE_M_109_T4	transfer					
MW_D_327_A1						
W_D_345_N6						
NE_B_678_L6	error404					
SW_D_467_Y3	syncon					
SW_D_448_O1	relationships	transfer	syncon			
SE_D_607_I9						
NE_D_374_L2	intuition	apply				
SE_D_642_T10	explain	word	diagram			
SE_B_13_M3	explain					
W_M_667_U9	intuition					
W_D_498_W9	diagram	Describe				
SW_D_333_D10	intuition					
MW_D_545_U7	syncon	predict	transfer			
MW_B_131_R10	explain	predict				
SW_D_454_X10	intuition					
W_D_49_Q5	syncon	predict				
NE_B_30_A3	intuition	modeling				
SE_B_174_Y5	diagram					
W_B_69_H4	intuition					
W_B_329_B2	intuition	syncon				
W_D_112_M3	word	diagram	explain	syncon		
MW_B_189_W5	transfer					
SE_B_196_R6	intuition					
W_B_582_V4	intuition	diagram	explain	unpaired		
W_D_112_J10						
W_D_494_M1	intuition	syncon				
W_D_493_F8	intuition	syncon				
W_M_63_W3	intuition	syncon				
SE_M_229_Y1	problem	Describe	explain			
SE_D_516_E1	syncon					
SE_B_355_S7	relationships					
MW_D_350_J8	explain	simplify	modeling			
MW_D_266_U9	intuition	predict	modeling			
SE_M_302_L4	intuition	relationships				
MW_B_102_U9	Describe	explain	modeling	predict	transfer	error404
SE_D_661_D2	intuition	paired				
NE_D_589_K9	explain	syncon				
NE_B_678_M7						
MW_B_120_N10	intuition	modeling				
SE_D_178_W9	intuition	transfer				
W_B_390_U7	relationships	diagram				
MW_M_371_V6	explain	Describe	predict	unpaired	Describe	teach
MW_D_549_Y7	intuition					

NE_D_532_Z4	syncon	intuition				
SW_D_308_Y7	intuition					
SW_D_468_B6	intuition	paired				
NE_B_104_D8	transfer	memorization	symbols			
MW_D_528_A9	intuition					
NE_B_340_L8	intuition	syncon	unpaired	relationships		
NE_D_375_Q7	unpaired	intuition				
MW_M_289_E1	paired	intuition				
NE_B_119_M9	intuition	syncon				
MW_D_653_W9	memorization	Describe	apply	transfer	problem	intuition
NE_D_374_J10	intuition	predict				
MW_M_141_O3	syncon	Explain	unpaired	diagram		
SW_M_469_F10	explain	syncon	unpaired	apply		
MW_D_555_N2	explain	relationships	paired			
MW_B_106_H2	intuition					
W_M_205_F10	intuition					
NE_B_11_I9	relationships	syncon	explain			
NE_B_442_C3	word	syncon				
MW_D_290_J6	intuition					
NE_B_383_A7	explain	intuition	modeling			
NE_D_43_B10						
NE_B_397_C5	relationships	intuition	syncon			
SE_B_13_N4	intuition					
W_M_389_P2	explain	intuition	transfer			
MW_D_545_Z2						
MW_M_289_D10	explain	word	syncon	transfer		
NE_B_164_I9	intuition	syncon				
NE_B_433_D8						
MW_D_542_R8	intuition					
NE_M_90_Q9	explain	relationships	predict			
MW_D_290_H4	syncon	intuition				
NE_B_348_C1	explain	modeling				
NE_D_43_F4	Error404	syncon	synmath			
MW_M_28_X10	syncon	predict				
MW_D_326_Q1	intuition					
MW_B_330_I9	transfer					
SW_D_408_B10	relationships	symbols	intuition			
NE_M_90_S1	paired	intuition				
W_M_60_G7	intuition	diagram				
SE_D_160_N8		intuition				
SE_B_13_L2	unpaired	relationships				
SW_M_453_S5	syncon	intuition				
MW_D_226_W9						
MW_B_184_O7	word	diagram				
SE_B_650_R4	intuition	modeling				
NE_D_589_L10	symbols	paired				
NE_D_347_W5	explain	Describe	word	teach		
#N/A	modeling					
W_D_495_C7	intuition					
W_D_619_O7	predict	unpaired	modeling	intuition		
SW_D_609_W3	syncon	predict				
W_D_470_V6	syncon					
NE_B_362_K5	word	diagram	explain			
SE_D_516_W3		syncon	problem			
SW_M_322_H2	Intuition					
NE_M_464_K9	transfer					
SE_M_662_K9		predict	unpaired	intuition		
W_D_498_E1	syncon	predict	explain			
MW_M_325_N8	syncon	explain	predict			
SE_M_229_A3	intuition					
MW_D_528_E3	explain					
W_D_619_H10	syncon	relationships				
SE_B_414_L10	syncon	diagram	explain			
NE_B_169_M3	explain	predict	modeling	intuition		
MW_D_542_C9	Error404					
W_D_493_B4	transfer					
NE_D_133_T2		transfer	explain			
W_M_667_X2	word	explain				
W_D_494_Z8		modeling				
NE_B_419_N2	word					
NE_M_296_C5	relationships	transfer	intuition			
W_M_388_I5	problem		relationships			
MW_B_12_K1	explain					
SE_M_109_S3	unpaired	relationships				
SW_M_386_C9	Describe					
SE_D_151_Z4	explain	predict				
SW_D_15_I5						
W_D_54_Q1	syncon					
SE_M_665_Q5	transfer					
MW_B_264_Q5		intuition				
NE_B_216_O5	error404					
MW_D_277_Y9	word	diagram				

MW_B_184_M5	explain	word	
SE_D_531_T8	Describe	diagram	intuition
MW_D_654_U3	word	describe	
MW_B_330_K1	intuition		
NE_D_347_Y7	intuition		
MW_D_625_V10	syncon	unpaired	intuition
MW_B_283_V2	relationships	intuition	transfer
SW_D_609_Y5	intuition		
SE_B_156_L6	syncon		
MW_M_291_X10	unpaired		
W_M_667_Y3	Describe	transfer	
NE_B_394_W9	explain	modeling	
W_D_494_D2	Describe		
SE_B_36_K3	word	diagram	unpaired
MW_D_577_F2	word	explain	
W_M_667_V10	explain	word	diagram

Participant	Mathematical Codes					
SE_D_135_D2	Symbols	unpaired				
W_D_497_U1	Symbols	relationships	algorithm			
W_D_294_A3	modeling	symbols				
NE_D_223_L8	synmath	relationships	paired	explain	apply	
MW_B_9_F6	Tool	algorithm	apply	modeling		
MW_B_238_M5						
W_D_470_I3	Symbols	algorithm				
MW_B_363_M7	Symbols	algorithm				
NE_B_282_U1	symbols	relationships	modeling			
MW_D_465_O3	paired	problem	intuition	algorithm		
MW_B_682_R2	apply	algorithm				
SW_D_408_W5	symbols	generate	relationships			
W_D_495_P10	error404					
NE_B_442_E5	symbols	apply	syncon			
W_M_62_N4	algorithm	problem				
NE_M_641_O5	predict	argument	generate	apply	syncon	
NE_D_439_S3	tool	symbols	intuition			
MW_D_331_T10	symbols	relationships				
SE_D_502_T2	explain	paired	predict	apply	memorization	interpret
MW_D_625_Y3	relationships	intuition				
NE_B_11_H8	error404	tool				
MW_D_527_W5	synmath	diagram	symbols	paired	algorithm	
MW_D_327_Z10	explain	symbols	argument			
NE_D_485_O5	intuition	paired				
W_B_592_T8	symbols	relationships	transfer	algorithm	explain	syncon
W_D_112_P6	symbols	relationships	algorithm			
W_D_49_Z4	tool	paired	relationships	syncon	simplify	
NE_B_147_S7	relationships	symbols				
NE_B_70_W9	explain	synmath	paired	symbols	relationships	apply
NE_B_601_V6	algorithm	intuition	paired	tool		
SE_B_352_P4	problem	apply	algorithm	symbols		
NE_D_581_O7	symbols	modeling	interpret	algorithm		
SE_M_665_O3	synmath	syncon	predict	paired	transfer	
NE_M_93_E3	algorithm					
SW_B_591_R6	symbols	algorithm				
MW_B_416_M1	diagram	symbols	relationships	apply		
NE_D_121_V8	algorithm	problem				
MW_D_625_Q5	relationships	symbols	apply			
SE_B_621_S1	error404					
NE_B_250_D2	synmath	predict	problem	apply	algorithm	
SE_D_517_M9	intuition	algorithm	tool			
NE_D_581_M5	symbols	intuition	algorithm			
MW_D_542_T10	Algorithm	Paired				
MW_B_122_C5	Intuition					
SE_B_13_P6	SynMath	SynCon	Paired			
SE_D_151_Y3	Relationships					
SE_D_548_O7	Argument	Explain	Symbols			
NE_B_377_T10	Symbols	Relationships	SynCon			
SE_B_569_Q1	Symbols	Algorithm	Relationships			
SE_B_149_V10	Symbols	Algorithm				
W_B_166_L2	SynMath	Algorithm				
W_B_592_V10	Symbols	Paired				
MW_D_528_B10	Word	Symbols				
MW_D_78_D6	Problem	Algorithm	Symbols	SynCon		
SE_D_502_Q9	Symbols	Paired	Explain	SynCon		
MW_D_577_D10	Symbols	SynCon	modeling			
MW_M_407_V4	Paired	SynMath	Predict	modeling		
NE_D_347_V4	Symbols	SynMath				
MW_B_627_E9	Symbols	Algorithm	Relationships	Apply	modeling	
NE_B_6_E5	Problem	SynCon				
NE_D_341_X10	Symbols					
NE_D_581_K3	Generate	modeling				
NE_D_485_K1	SynMath	Apply	Predict	Symbols		
NE_B_649_Q3	Algorithm					
W_D_49_X2						

W_D_633_N8	Algorithm	symbols					
W_M_55_V6	SynMath	Algorithm	Symbols	Apply			
NE_B_70_K7	Paired	Transfer	Symbols	Algorithm			
MW_M_679_N8	Intuition	Symbols	Algorithm	Problem			
NE_B_399_H10	Symbols	Algorithm	modeling				
SW_D_467_V10	Symbols	Algorithm					
NE_D_614_A7	Symbols						
W_M_205_G1	Tool	Transfer	Describe	intuition			
W_D_470_P10	Symbols	Paired					
MW_B_669_A5	Symbols	Modeling	Explain	Predict	Relationships		
W_D_496_B2	Algorithm	Explain	modeling				
NE_D_512_D4	Paired	SynMath					
NE_B_677_J4	SynMath	Relationships	modeling				
SW_D_608_O5	Argument	Tool					
NE_B_179_E7	Modeling	Symbols	predict	Apply			
MW_M_576_H8	Symbols	Algorithm	Relationships				
SE_B_569_R2	Symbols	Algorithm	Modeling	Problem			
SE_B_354_Q5	Explain	Symbols					
MW_M_546_E7							
NE_B_263_P4	Symbols	Relationships	Predict	Apply			
NE_D_537_H8	Apply	Symbols					
NE_B_399_I1	Symbols	Algorithm	diagram	SynMath			
MW_D_577_R8	SynMath	Predict	Apply				
NE_M_93_Z8	Error404						
SE_D_100_N2	Algorithm	SynMath	Problem	Relationships	Transfer	Intuition	Paired
SE_D_647_M9	Error404						
NE_B_634_O9	Algorithm	Symbols	Explain	SynCon			
NE_D_535_S3	Generate	Symbols					
NE_D_486_Q7	Intuition						
SW_M_386_D10	Symbols	Describe					
MW_D_549_W5	Algorithm						
MW_D_278_I9	Algorithm	Symbols					
NE_D_51_G1	Symbols	Apply					
MW_B_127_I1	Modeling	Algorithm					
W_B_339_K7	Symbols	Relationships	Modeling				
MW_D_666_R6	Symbols	Relationships	Intuition				
SW_D_466_R6	Error404						
SE_B_221_F2	Symbols	Relationships					
SE_B_572_Z10	Symbols	Problem	Modeling				
NE_B_651_T6	Symbols	Algorithm	Relationships				
W_M_60_F6	Paired	SynCon	SynMath				
NE_D_341_T6	Symbols	Problem					
W_B_592_S7	Symbols	Tool					
MW_B_148_T8	Symbols	Algorithm	Paired	Interpret	modeling		
W_D_470_L6	Symbols	Tool	SynCon				
SE_D_462_E3	Apply	Symbols	Paired	Problem	intuition		
SW_D_520_U7	Symbols	Modeling	Apply				
MW_D_78_A3							
SE_D_288_Z6	Algorithm	SynMath					
NE_D_92_W5	explain	synmath	problem	modeling			
MW_B_261_O3	symbols	unpaired					
SE_M_109_T4	algorithm	problem	symbols	tool			
MW_D_327_A1							
W_D_345_N6							
NE_B_678_L6	relationships	apply	generate	intuition			
SW_D_467_Y3	synmath	symbols	algorithm				
SW_D_448_O1	algorithm	interpret					
SE_D_607_I9	intuition						
NE_D_374_L2	symbols	modeling	tool				
SE_D_642_T10	symbols	diagram	algorithm				
SE_B_13_M3	tool	explain	apply				
W_M_667_U9							
W_D_498_W9	generate	predict	modeling				
SW_D_333_D10	synmath	predict					
MW_D_545_U7	symbols	intuition					
MW_B_131_R10	symbols	tool	transfer	relationships	paired	unpaired	
SW_D_454_X10	symbols						
W_D_49_Q5	synmath	predict					
NE_B_30_A3	relationships	intuition					
SE_B_174_Y5	intuition	symbols					
W_B_69_H4	symbols	interpret	tool				
W_B_329_B2	unpaired						
W_D_112_M3	symbols	diagram					
MW_B_189_W5	relationships	intuition	paired				
SE_B_196_R6	explain	intuition	unpaired				
W_B_582_V4	unpaired	symbols	explain				
W_D_112_J10	symbols	transfer	unpaired				
W_D_494_M1	tool	symbols	paired				
W_D_493_F8	intuition						
W_M_63_W3	synmath	unpaired					
SE_M_229_Y1	algorithm	symbols					
SE_D_516_E1	synmath	algorithm					

SE_B_355_S7	modeling	algorithm	problem	symbols	relationships
MW_D_350_J8	symbols	explain	algorithm	modeling	
MW_D_266_U9	algorithm	predict			
SE_M_302_L4	intuition	algorithm			
MW_B_102_U9	algorithm	unpaired	modeling		
SE_D_661_D2	Describe	explain			
NE_D_589_K9	problem	synmath			
NE_B_678_M7					
MW_B_120_N10	intuition	symbols	syncon		
SE_D_178_W9	tool	algorithm	unpaired	intuition	
W_B_390_U7	algorithm	symbols			
MW_M_371_V6	modeling	symbols	synmath	unpaired	apply
MW_D_549_Y7	intuition	paired			
NE_D_532_Z4	intuition	paired			
SW_D_308_Y7	tool	memorization	problem		
SW_D_468_B6	intuition	paired			
NE_B_104_D8	symbols	transfer	memorization		
MW_D_528_A9	symbols	modeling			
NE_B_340_L8	symbols	apply	algorithm		
NE_D_375_Q7	symbols	predict			
MW_M_289_E1	intuition				
NE_B_119_M9	symbols	algorithm	interpret	modeling	
MW_D_653_W9	modeling	problem	algorithm		
NE_D_374_J10	symbols	interpret			
MW_M_141_O3	Explain	interpret	symbols	synmath	
SW_M_469_F10	explain	relationships	algorithm		
MW_D_555_N2	explain	relationships	symbols		
MW_B_106_H2	symbols	paired	algorithm		
W_M_205_F10	intuition				
NE_B_11_I9	paired	synmath	relationships	simplify	
NE_B_442_C3	algorithm	diagram			
MW_D_290_J6	intuition	symbols			
NE_B_383_A7	explain	algorithm	memorization	modeling	
NE_D_43_B10	synmath	predict			
NE_B_397_C5	synmath	relationships	intuition		
SE_B_13_N4	intuition				
W_M_389_P2	symbols	word	predict		
MW_D_545_Z2					
MW_M_289_D10	algorithm	synmath	problem		
NE_B_164_I9		symbols	intuition	describe	
NE_B_433_D8					
MW_D_542_R8	Symbols	paired			
NE_M_90_Q9	Generate	symbols	intuition		
MW_D_290_H4	symbols	problem	intuition		
NE_B_348_C1	predict	symbols	modeling		
NE_D_43_F4	synmath	symbols	intuition		
MW_M_28_X10	synmath	predict			
MW_D_326_Q1	synmath	intuition			
MW_B_330_I9	predict	symbols			
SW_D_408_B10	symbols	relationships			
NE_M_90_S1	symbols	transfer			
W_M_60_G7		tool			
SE_D_160_N8	intuition				
SE_B_13_L2	relationships				
SW_M_453_S5	symbols				
MW_D_226_W9					
MW_B_184_O7	tool	word	diagram		
SE_B_650_R4	predict	syncon	modeling		
NE_D_589_L10	algorithm	synmath	predict		
NE_D_347_W5	synmath	symbols			
#N/A	symbols	modeling			
W_D_495_C7	symbols	problem			
W_D_619_O7	predict	modeling			
SW_D_609_W3	paired	explain			
W_D_470_V6	symbols	algorithm			
NE_B_362_K5	symbols				
SE_D_516_W3	Symbols				
SW_M_322_H2	Symbols				
NE_M_464_K9	problem				
SE_M_662_K9	symbols	predict			
W_D_498_E1	synmath	predict	explain		
MW_M_325_N8	symbols	algorithm			
SE_M_229_A3	relationships	generate			
MW_D_528_E3	interpret	predict			
W_D_619_H10	predict	symbols	synmath		
SE_B_414_L10	synmath	symbols			
NE_B_169_M3	paired	symbols			
MW_D_542_C9	symbols				
W_D_493_B4	synmath				
NE_D_133_T2	symbols	predict			
W_M_667_X2	synmath	predict	symbols	modeling	
W_D_494_Z8	symbols	tool	algorithm		

NE_B_419_N2	symbols				
NE_M_296_C5	symbols				
W_M_388_I5	symbols	problem			
MW_B_12_K1	synmath	symbols	modeling		
SE_M_109_S3	simplify	symbols			
SW_M_386_C9	modeling				
SE_D_151_Z4	symbols	predict			
SW_D_15_I5					
W_D_54_Q1	synmath	symbols	algorithm		
SE_M_665_Q5	intuition	paired			
MW_B_264_Q5	algorithm				
NE_B_216_O5	error404				
MW_D_277_Y9	algorithm				
MW_B_184_M5	explain	synmath	symbols		
SE_D_531_T8	relationships	symbols			
MW_D_654_U3	symbols	describe			
MW_B_330_K1	symbols				
NE_D_347_Y7	symbols				
MW_D_625_V10	symbols	algorithm			
MW_B_283_V2	algorithm	symbols	unpaired		
SW_D_609_Y5	symbols	paired			
SE_B_156_L6	synmath	apply			
MW_M_291_X10	symbols				
W_M_667_Y3	symbols	algorithm			
NE_B_394_W9	interpret	symbols			
W_D_494_D2	symbols				
SE_B_36_K3	paired	symbols			
MW_D_577_F2	synmath	algorithm			
W_M_667_V10	syncon	synmath	symbols	word	diagram

S.5: KNOWLEDGE DOMAIN DATA

A – US Region	B – Highest Degree	C – Carnegie Classification	D – Research	E – Last Time Taught	F – Number of Times Taught	#1-20
West 1 Midwest 2 Southeast 3 Northeast 4 Southwest 5	Bachelors 1 Masters 2 PHd 3	R1 - 1 R2 - 2 R3 - 3 Diverse Fields -4 Arts & science -5 M1 - 6 M2 - 7 M3 - 8 D/PU - 9 Special focus - 10	1 = Experimental, 2 = Experimental/Physical Chemistry Education, 3 = Experimental/Theoretical/Computational, 4 = Experimental/Theoretical/Computational/Physical Chemistry Education, 5 = Does not Perform Research, 6 = Physical Chemistry Education, 7 = Theoretical/Computational 8 = Theoretical/computational/Physical Chemistry Education	*1 = never, 2 = Within the last year, 3 = (1-5) Years ago, 4 = (6-10) Years ago, 5 = (11-15) Years ago, 6 = (16-20) Years ago, 7 = more than 20 years ago*	*1 = never, 2 = (1-5) times, 3 = (6-10) times, 4 = (11-15) times, 5 = (16-20) times, 6 = more than times*	*survey items 1-20 1 = mostly conceptual, 2= mostly mathematical, 3 = equally conceptual and mathematical 4 = other*

Participant	A	B	C	D	E	F	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
SE_D_135_D2	3	3	1	1	2	3								1				1	1		3				1	
W_D_497_U1	1	3	1	1	6	4					2				1	3	3					4				
W_D_294_A3	1	3	1	7	1	1	4	2	1											3				3		
NE_D_223_L8	4	3	1	1	5	2				3			3								1	3		1		
MW_B_9_F6	2	1	4	8	2	3	1				3				1		1		1							
MW_B_238_M5	2	1	4																							
W_D_470_I3	1	3	1	1	5	3			1							1		3							3	1
MW_B_363_M7	2	1	5	7	2	4					1		1	2	1					1						
NE_B_282_U1	4	1	6	3	2	3			2			1						2							3	1
MW_D_465_O3	2	3	2	7	2	2		3				1			1		1						1			
MW_B_682_R2	2	1	5	6	2	3	1				3		1											3	1	
SW_D_408_W5	5	3	2	7	4	2													1	1	3	2		3		
W_D_495_P10	1	3	1	1	5	6				1	3	3		3						1						
NE_B_442_E5	4	1	5	1	5	4		3					3	1				3					3			
W_M_62_N4	1	2	6	7	2	3	1		1										1			3				3
NE_M_641_O5	4	2	2	7	2	3		2			1			2			1			1						
NE_D_439_S3	4	3	1	7	3	2	1			1									1		2	3				
MW_D_331_T10	2	3	2	1	3	2				3					4				1		1				1	
SE_D_502_T2	3	3	1	1	1	1		3		3						1		3						1		
MW_D_625_Y3	2	3	1	7	2	2				3									1			3		3		1
NE_B_11_H8	4	1	5	1	1	1				1						1		1					1	1		
MW_D_527_W5	2	3	1	7	2	2	3					4			1			4							4	
MW_D_327_Z10	2	3	2	7	2	2			1					3			1	1					3			
NE_D_485_O5	4	3	1	1	3	2			1						1	1						3		2		
W_B_592_T8	1	1	2	1	2	4		2	1							4					1				1	
W_D_112_P6	1	3	1	7	2	3		2					3							1			3	3		
W_D_49_Z4	1	3	2	1	5	2		3					3								3		3		3	
NE_B_147_S7	4	1	5	7	2	6						1			1		1				3		2			
NE_B_70_W9	4	1	6	1	2	2	1				2					1								2		3
NE_B_601_V6	4	1	6	6	2	6			1					2		1	1			1						
SE_B_352_P4	3	1	6	7	2	4							2				1		1				1			1
NE_D_581_O7	4	3	1	1	2	2					2				1						1				1	1
SE_M_665_O3	3	2	9	1	2	3	1				3			3	1						1					
NE_M_93_E3	4	2	6	1	3	2			2							4	3								2	3
SW_B_591_R6	5	1	6	7	2	3		2			3	3		1			1									
MW_B_416_M1	2	1	6	6	2	4		2			1				2			3			1					
NE_D_121_V8	4	3	1	1	4	2	1		1		1											3				2
MW_D_625_Q5	2	3	1	1	3	6		1						3							1		1			1
SE_B_621_S1	3	1	9	3	2	4	1	1		1												1			1	
NE_B_250_D2	4	1	7	8	2	4	1						3				1	1	1							
SE_D_517_M9	3	3	1	1	2	2			1			1	1						1			3				

NE_D_581_M5	4	3	1	7	3	3											1		3		3		1	3		
MW_D_542_T10	2	3	1	7	7	3	1			1			1						1						1	
MW_B_122_C5	2	1	9	7	2	5			1	1		1			1							3				
SE_B_13_P6	3	1	6	1	4	2					2	1		2											3	3
SE_D_151_Y3	3	3	1	7	3	2			1				3		1	1				1						
SE_D_548_O7	3	3	1	7	2	3	3						3						1			1		3		
NE_B_377_T10	4	1	5	1	3	6				1		4								4					1	1
SE_B_569_Q1	3	1	6	8	3	6					2	4		2		1										1
SE_B_149_V10	3	1	9	2	2	2	1	2	3			1									3					
W_B_166_L2	1	1	5	4	2	3	1							4			1			4			4			
W_B_592_V10	1	1	2	7	2	3					3	1					1	2				3				
MW_D_528_B10	2	3	1	7	3	2									3	1				3	3					3
MW_D_78_D6	2	3	1	7	2	2							3							1	1		1		1	
SE_D_502_Q9	3	3	1	6	1	1	1			2									1		2		2			
MW_D_577_D10	2	3	1	1	2	2							3					1	3			3			1	
MW_M_407_V4	2	2	9	1	3	5			3		1			3					1	1						
NE_D_347_V4	4	3	1	7	2	5							3	3	1		1						3			
MW_B_627_E9	2	1	6	4	2	5				3		1					3				4	2				
NE_B_6_E5	4	1	5	1	2	3	3									1				1			3	2		
NE_D_341_X10	4	3	1	7	1	1					2					1	4							3		1
NE_D_581_K3	4	3	1	3	3	2		2									3	1	1				1			
NE_D_485_K1	4	3	1	7	2	2						1		3			1					3			3	
NE_B_649_Q3	4	1	5	3	2	5	1		1									1				2			1	
W_D_49_X2	1	3	2																							
W_D_633_N8	1	3	2	1	4	2		3	3										1	1	1					
W_M_55_V6	1	2	6	7	2	5									1			2		1		1	3			
NE_B_70_K7	4	1	6	1	2	2				1						1				1	1			1		
MW_M_679_N8	2	2	8	7	3	2	1			1	3		3												1	
NE_B_399_H10	4	1	5	6	7	3	1						2			2									1	1
SW_D_467_V10	5	3	1	7	2	5		2				1					1							2		3
NE_D_614_A7	4	3	10	7	2	3					1			3	1		1		1							
W_M_205_G1	1	2	2	1	2	6	1				3				1	1		1								
W_D_470_P10	1	3	1	1	2	2			3					2		1			1		1					
MW_B_669_A5	2	1	5	1	2	5				2			1										1	2		1
W_D_496_B2	1	3	1	1	2	2			2	1		1			1										3	
NE_D_512_D4	4	3	1	7	2	2			3		3			3	1			3								
NE_B_677_J4	4	1	6	7	2	3	3					3	3						1						3	
SW_D_608_O5	5	3	1	1	2	3	1						1				1			1						1
NE_B_179_E7	4	1	5	5	2	6	1									1				1					1	1
MW_M_576_H8	2	2	6	1	3	4						4		4						4			4		4	
SE_B_569_R2	3	1	6	7	3	3		2								1				3				1		1
SE_B_354_Q5	3	1	5	7	2	2	2												1			2	3		2	
MW_M_546_E7	2	2	7																							

NE_B_263_P4	4	1	5	1	3	5						1	2								3	3			3	
NE_D_537_H8	4	3	1	5	4	5				3		1				1						2				2
NE_B_399_I1	4	1	5	1	3	2		2			3							2		1					3	
MW_D_577_R8	2	3	1	7	3	2				1				3	1			2	1							
NE_M_93_Z8	4	2	6	1	3	3				1	1		1		1					1						
SE_D_100_N2	3	3	1	7	4	2		2			2				1	1								3		
SE_D_647_M9	3	3	2	7	2	3		3								3	3					3			3	
NE_B_634_O9	4	1	5	1	2	6		1							1			2	1				4			
NE_D_535_S3	4	3	1	1	1	1			1			3	1											1	1	
NE_D_486_Q7	4	3	1	7	2	5						1	1					4		1						1
SW_M_386_D10	5	2	9	7	1	1	1		3				2		1							2				
MW_D_549_W5	2	3	1	7	2	2		2	1							1				1						3
MW_D_278_I9	2	3	2	7	2	3				3	3	3						1							1	
NE_D_51_G1	4	3	5	7	2	6	3								1		1				1			1		
MW_B_127_I1	2	1	5	1	2	2						1	3				1				1			3		
W_B_339_K7	1	1	7	1	2	3				3					1	1				3					1	
MW_D_666_R6	2	3	2	3	2	3			1	1				3			1				1					
SW_D_466_R6	5	3	1	3	2	3			4	1						4		1								4
SE_B_221_F2	3	1	6	1	2	6			1		1			1		1								1		
SE_B_572_Z10	3	1	9	1	2	2		4					3						1	1	1					
NE_B_651_T6	4	1	5	7	2	3	1							2	1								1		2	
W_M_60_F6	1	2	6	3	3	6				1	3		3				1									1
NE_D_341_T6	4	3	1	1	1	1			1		1				1	1										1
W_B_592_S7	1	1	2	1	1	1			3					2		2			1		3					
MW_B_148_T8	2	1	6	7	2	6					1	1					3					3		3		
W_D_470_L6	1	3	1	1	2	5				1		1					1		3				1			
SE_D_462_E3	3	3	1	7	3	3							1	3				1			1	3				
SW_D_520_U7	5	3	1	5	1	1							3	2				3						2	1	
MW_D_78_A3	2	3	1																							
SE_D_288_Z6	3	3	1	7	2	3	2			1							1			4						1
NE_D_92_W5	4	3	6	7	2	2	3					1			1			1				3				
MW_B_261_O3	2	1	5	1	2	5		2												1			3	1	1	
SE_M_109_T4	3	2	2	7	2	2			3						1				1	1	1					
MW_D_327_A1	2	3	2																							
W_D_345_N6	1	3	2																							
NE_B_678_L6	4	1	5	7	3	4		2	1														2		1	1
SW_D_467_Y3	5	3	1	7	4	2					3	4								1	3			3		
SW_D_448_O1	5	3	1	7	1	1	1			3				3	1	1										
SE_D_607_I9	3	3	1	7	3	2		2						3					1				1	1		
NE_D_374_L2	4	3	1	7	3	2							1	3			3						1	3		
SE_D_642_T10	3	3	1	1	2	2				1						1				3	3				1	
SE_B_13_M3	3	1	6	7	2	2	1		1		2									3						2
W_M_667_U9	1	2	6	1	4	4		1	1		1							3	3							
W_D_498_W9	1	3	1	1	3	2							3			1		1				1			1	
SW_D_333_D10	5	3	1	7	3	2	1	2			3	1										2				

MW_D_545_U7	2	3	1	7	4	2				1				3			1						1	3		
MW_B_131_R10	2	1	9	8	2	3		2						3								3	3		3	
SW_D_454_X10	5	3	1	7	1	1			1		1									1	3					1
W_D_49_Q5	1	3	2	1	1	1						3			1		1		1					2		
NE_B_30_A3	4	1	5	1	2	6					3					1	1	3			3					
SE_B_174_Y5	3	1	5	3	1	1	3			3			3			4		3								
W_B_69_H4	1	1	6	4	2	4	1												1		1		1	1		
W_B_329_B2	1	1	5	6	2	3	3			3		3	3											2		
W_D_112_M3	1	3	1	1	3	4								2						1		2	3		3	
MW_B_189_W5	2	1	6	3	3	2				1	1				3			1							1	
SE_B_196_R6	3	1	7	7	2	2	3					3	3				1									2
W_B_582_V4	1	1	7	1	2	6		2	1										1		3			3		
W_D_112_J10	1	3	1	1	1	1								2	1				1		3				3	
W_D_494_M1	1	3	1	7	3	2					1					1		1				1		1		
W_D_493_F8	1	3	1	7	3	4	3		3								3						1			3
W_M_63_W3	1	2	6	7	2	4		2		3		1	3							1						
SE_M_229_Y1	3	2	2	1	2	3		3	3									2	1							1
SE_D_516_E1	3	3	1	1	5	2					1		1				1								1	3
SE_B_355_S7	3	1	5	1	3	4				3						3	1						1			3
MW_D_350_J8	2	3	1	3	1	1	1					4				3				1			4			
MW_D_266_U9	2	3	2	1	2	2			3	3								3				3		2		
SE_M_302_L4	3	2	6	3	3	3			1				1	3					1	1						
MW_B_102_U9	2	1	5	2	2	6		3						1	4				1		1					
SE_D_661_D2	3	3	1	1	2	3					3	3					1	3			3					
NE_D_589_K9	4	3	1	1	1	1				1					1							3	3			1
NE_B_678_M7	4	1	5																							
MW_B_120_N10	2	1	5	4	2	5	1					1			1	1				1						
SE_D_178_W9	3	3	1	5	3	2			1	1											1			3	1	
W_B_390_U7	1	1	9	1	2	3					2			3			1					2	1			
MW_M_371_V6	2	2	10	7	3	3		3					2					2	1							1
MW_D_549_Y7	2	3	1	1	3	3	1		1			3	2									3				
NE_D_532_Z4	4	3	2	7	3	3				3	4					1			1							4
SW_D_308_Y7	5	3	8	6	2	5				1	1		3			3										1
SW_D_468_B6	5	3	2	7	3	6								3	3			1						2	3	
NE_B_104_D8	4	1	5	1	2	2		1		1	1					1	1									
MW_D_528_A9	2	3	1	1	3	4			2			1		3	1					1						
NE_B_340_L8	4	1	8	1	3	4		1									3		1		1			3		
NE_D_375_Q7	4	3	2	3	1	1	3											2				3	2		1	
MW_M_289_E1	2	2	9	1	2	6				2	2	1		3						1						
NE_B_119_M9	4	1	5	1	2	2							3			1		3				3		1		
MW_D_653_W9	2	3	1	1	2	2	1				3				1			1					1			
NE_D_374_J10	4	3	1	7	2	2				4		1		2										1		3
MW_M_141_O3	2	2	6	1	3	2		2	1				2			3						1				

SW_M_469_F10	5	2	2	7	2	4				4									1				1		2	1
MW_D_555_N2	2	3	1	1	2	3						2			1		1	3			4					
MW_B_106_H2	2	1	5	1	2	3	3				3			1						1				2		
W_M_205_F10	1	2	2	1	2	5		1				1						2					1	2		
NE_B_11_I9	4	1	5	3	2	5					1		3	4	1					1						
NE_B_442_C3	4	1	5	1	2	4	1			3							1				1					3
MW_D_290_J6	2	3	2	4	4	2	1	2												1		3	3			
NE_B_383_A7	4	1	5	2	2	6			3	3	3	1			1											
NE_D_43_B10	4	3	1	7	2	4	1				1									1	1				1	
NE_B_397_C5	4	1	5	7	2	2		1				1	1			1							1			
SE_B_13_N4	3	1	6	7	2	4	3						2							1		3	1			
W_M_389_P2	1	2	6	7	2	2		1	1	2					1				1							
MW_D_545_Z2	2	3	1																							
MW_M_289_D10	2	2	9	1	2	4						1				1	1							2		1
NE_B_164_I9	4	1	2	1	2	2		2	1		3										1		1			
NE_B_433_D8	4	1	6																							
MW_D_542_R8	2	3	1	1	1	1				1							1			1		3		1		
NE_M_90_Q9	4	2	6	3	3	2				1				3	1		1									2
MW_D_290_H4	2	3	2	7	3	4	1						1											1	1	1
NE_B_348_C1	4	1	8	3	2	4		2						3						1			1			1
NE_D_43_F4	4	3	1	5	1	1		2				3		3				3			3					
MW_M_28_X10	2	2	2	1	3	2					1			3	1				1						1	
MW_D_326_Q1	2	3	1	7	4	4	3	2										2		1	1					
MW_B_330_I9	2	1	4	7	1	1					1				1					1		3			1	
SW_D_408_B10	5	3	2	7	2	2	3	1		4					1						1					
NE_M_90_S1	4	2	6	7	2	2						1				4					2			1	3	
W_M_60_G7	1	2	6	1	2	2				3		3					1			1				2		
SE_D_160_N8	3	3	2	2	2	4			1			3			1	3							1			
SE_B_13_L2	3	1	6	1	3	2	4									1		4			4					1
SW_M_453_S5	5	2	2	1	3	2		1										1	1		1			3		
MW_D_226_W9	2	3	1																							
MW_B_184_O7	2	1	6	1	3	3			3	3	3									3						3
SE_B_650_R4	3	1	5	7	3	6	1					3	1		3	1										
NE_D_589_L10	4	3	1	1	2	2								3				3		1		3			1	
NE_D_347_W5	4	3	1	1	2	2		4										2			3	2	1			
	3	2	7	8	3	6								3			1		1					3	1	
W_D_495_C7	1	3	1	7	1	1									4		3			1		3				1
W_D_619_O7	1	3	1	3	2	4							1	2			4			1					1	
SW_D_609_W3	5	3	1	1	2	3			1	1			3										1	1		
W_D_470_V6	1	3	1	1	2	3	3	2										2				3		3		
NE_B_362_K5	4	1	6	4	2	6			3				2							3	1					2
SE_D_516_W3	3	3	1	1	3	4				2	1		3				1	2								
SW_M_322_H2	5	2	2	7	2	2				1	1	1						3					4			

NE_M_464_K9	4	2	6	3	2	6					3	1							1		3					1
SE_M_662_K9	3	2	6	1	2	5								3		1	1		1						1	
W_D_498_E1	1	3	1	1	4	2					3		3				1		1				1			
MW_M_325_N8	2	2	7	7	2	6		3					2					2		1						1
SE_M_229_A3	3	2	2	1	2	4			1		1	1									1	4				
MW_D_528_E3	2	3	1	7	2	4					3	1		2						1		3				
W_D_619_H10	1	3	1	7	3	3		4					3		1			3					4			
SE_B_414_L10	3	1	5	7	2	2			3							1	1				4				3	
NE_B_169_M3	4	1	5	1	3	5		2							1				1	1						1
MW_D_542_C9	2	3	1	1	4	2						1						2			1	1		4		
W_D_493_B4	1	3	1	1	2	4	3			1					3								1	3		
NE_D_133_T2	4	3	1	7	2	6			1	3					1	1							1			
W_M_667_X2	1	2	6	7	2	2				1	3						1						1		3	
W_D_494_Z8	1	3	1	1	1	1		2			3						1	3					1			
NE_B_419_N2	4	1	5	1	2	5				3											1	3			1	1
NE_M_296_C5	4	2	2	7	2	2	1		1					3	1				1							
W_M_388_I5	1	2	6	7	2	2				1				4		1				1						3
MW_B_12_K1	2	1	9	4	2	3	1		3			1						2							1	
SE_M_109_S3	3	2	2	1	2	2					3		1				1		1			1				
SW_M_386_C9	5	2	9	4	2	5		2							2						3		3	2		
SE_D_151_Z4	3	3	1	7	3	2							3				1	2			1		3			
SW_D_15_I5	5	3	1																							
W_D_54_Q1	1	3	1	7	6	3	1				1				1	1			1							
SE_M_665_Q5	3	2	9	1	4	5			3					3										3	3	3
MW_B_264_Q5	2	1	4	2	2	5		3		1		1								1		2				
NE_B_216_O5	4	1	6	7		3			1			1									1		1	1		
MW_D_277_Y9	2	3	1	7		3	1												1		1			1		4
MW_B_184_M5	2	1	6	7		3		3				1						3		1		3				
SE_D_531_T8	3	3	1	3		2							2	2	1				1				1			
MW_D_654_U3	2	3	1	7		2				1		1	3		1							3				
MW_B_330_K1	2	1	4	1		3					3				1		3	3		1						
NE_D_347_Y7	4	3	1	7		1				1				3					1						1	1
MW_D_625_V10	2	3	1	1		3								3			1		3		1		1			
MW_B_283_V2	2	1	4	2		3	4					1	3			1								2		
SW_D_609_Y5	5	3	1	1		6				1			2	3		1						3				
SE_B_156_L6	3	1	7	1		3	1	3				1					1		1							
MW_M_291_X10	2	2	7	7		4			3														1	2	1	1
W_M_667_Y3	1	2	6	7		3			3			2		2		1										1
NE_B_394_W9	4	1	6	7		4							1				1		1	1		3				
W_D_494_D2	1	3	1	1		1	3			1								1					1	1		
SE_B_36_K3	3	1	5	1		6					1						1				1	1				1
MW_D_577_F2	2	3	1	7		1										1			1	1			1	3		

W_M_667_V10	1	2	6	7		3	1	3	3			1	3													