A Quantum Chemistry Concept Inventory for Physical Chemistry Classes

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Ⓢ *Supporting Information*

ABSTRACT: A 14-item, multiple-choice diagnostic assessment tool, the quantum chemistry concept inventory or QCCI, is presented. Items were developed based on published student misconceptions and content coverage and then piloted and used in advanced physical chemistry undergraduate courses. In addition to the instrument itself, data from both a pretest, prior to a semester of instruction, and a post-test, after a semester of instruction, are provided. These data suggest that the QCCI is capable of measuring the variation of student conceptual understanding of quantum mechanics in the context of a physical chemistry course and that the instrument is sensitive to gains in student understanding that result from direct instruction in the topic, even when that instruction has a significant mathematical component as is common for this course.

KEYWORDS: *Upper-Division Undergraduate, Physical Chemistry, Misconceptions/Discrepant Events, Testing/Assessment*

■ INTRODUCTION

To the extent that meaningful learning is taking place,[1,2] students in upper level undergraduate courses such as physical chemistry should be building knowledge upon foundations built in earlier courses in college. This premise is a core aspect of constructivism, a framework that helps organize a number of research efforts in science education.[3] A key idea is that learning in the sciences is contingent on a number of factors including prior knowledge.[4] Unsurprisingly, the fidelity of this prior knowledge is not uniformly robust, and instructors in upper-level courses can benefit from having a better estimate of student conceptual understanding upon entering that course. In this sense, an easily administered and scored assessment instrument for quantum chemistry represents a step that may improve instruction in upper level physical chemistry. This manuscript reports on the development and use of such an instrument.

There has been some significant work on student misconceptions related to topics that are commonly taught in the quantum chemistry component of physical chemistry. Of course, many of the core concepts in quantum chemistry such as chemical bonding or orbitals are treated earlier in the curriculum as well. Student conceptions of atoms play a key role in their understanding of the particulate nature of matter, and some quantum concepts are apparent early in the study of chemistry.[5] Tsaparlis and co-workers have considered the role of quantum concepts in earlier courses in a series of papers.[6−9] Taber has focused attention on student understanding of atomic and molecular orbitals within the context of the concept of quanta.[10−12] Galley found that students in introductory

physical chemistry courses enter the course believing that bond breaking is an exothermic process.[13] A number of studies have considered bonding concepts and misconceptions among more novice students,[14−21] and it is reasonable to expect that some misconceptions that are held in these earlier stages of learning are robust enough to persist into upper-level courses. For example, student misconceptions about bond polarity,[16,19] transfer of electrons in ionic bond formation rather than the attraction of ions,[15,20] and interpretation of covalent bonds as literal "sticks" may hinder student understanding of the role of molecular orbitals in bonding.[16,20] Quantitative studies have determined the prevalence of bonding misconceptions among more novice students through concept inventories, which allow instructors to quickly assess student understanding.[14,22−24] However, none of the inventories appears to have been used with higher-level students.

For students in courses with more advanced treatments of quantum mechanics, the majority of research arises in the physics education research literature. Several aspects, often with a mathematical emphasis, were noted in early efforts to identify student misconceptions in modern physics classes.[25] Singh and co-workers have also carried out a number of studies investigating student mathematical facility within quantum mechanics and teaching interventions designed to address these difficulties.[26−29] There have been several concept inventory style instruments devised in physics as well, again with

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significant emphasis on mathematical concepts. An initial instrument emphasized a number of aspects of quantum mechanics including visualization of wave functions.[30] A 25-item instrument was designed to include both interpretive items (that depend on the interpretation of the nature of quantum mechanics) and noninterpretive items that have identifiable correct answers.[31] A second instrument with a significant emphasis on the concept of tunneling has also been described.[32] Finally, Brown[33] has included items to assess student conceptual understanding in both quantum mechanics and physics as part of recently published thesis work. These studies provide insight into a number of commonly held student misconceptions, but the emphasis in the quantum treatment in physical chemistry is not highly aligned with the content in these instruments. Thus, a new instrument with a more chemistry orientation was deemed important to have, but these previous studies were used in the development of several of the items in the inventory reported here.

■ INSTRUMENT DEVELOPMENT

The motivation for the development of the Quantum Chemistry Concept Inventory (QCCI) was to measure conceptual understanding of the topics commonly taught in the quantum portion of the junior-level physical chemistry class that is common in the U.S. undergraduate curriculum. Prior to the junior-level physical chemistry class, the typical U.S. undergraduate student takes a general or introductory chemistry course that includes the quantum chemistry concepts: atoms, electrons, valence bond theory, and electromagnetic radiation. The introductory course is typically followed by organic, analytical, and potentially inorganic chemistry courses. Other typically required courses are two semesters each of calculus and calculus-based physics. These courses reflect the requirements for undergraduate program approval by North American professional societies.[34,35] The results from a pilot study seemed to indicate that students' misconceptions remain for some topics even after instruction in a physical chemistry course. Additionally, the QCCI from the pilot study displayed positive characteristics prompting further testing and refinement. Thus, a larger study, which included administering the QCCI to students from across the U.S. and Canada, was conducted.

The QCCI was designed with an eye toward content coverage more than an interest in identifying misconceptions that parallel those found earlier in the chemistry curriculum or in physics courses for quantum mechanics.

The key content coverage assumed in this study includes:

(1) Observations leading to quantum models for matter
(2) Development of the Schrödinger equation
(3) Particle in a box
(4) Harmonic oscillator
(5) Rigid Rotor
(6) Spectroscopic applications of simple models
(7) Hydrogen atoms
(8) Variational methods
(9) Many-electron systems and Hartree−Fock
(10) Molecular orbital theory
(11) Diatomic molecules
(12) Larger molecules

The overall approach within this content list utilizes significant mathematical treatment as well as conceptual understanding. Modest student facility with mathematics in the context of this type of physical chemistry course has been noted previously.[36,37] In addition, a student mindset that success in quantum mechanics requires an emphasis on mathematical problem solving has been characterized.[38] There may, therefore, be a tendency for instruction to focus on helping students simultaneously acquire the math skills used in topics such as quantum chemistry and the application of those skills to problems of chemical interest. If students struggle significantly with the mathematics itself, many instructors will provide additional assistance, and time on task, with the math content at the possible expense of the development of conceptual chemical understanding. It may be argued that such instructional decisions benefit from enhanced information, and therein lies a key motivation for the development of an instrument to measure conceptual understanding of students in quantum chemistry. Mathematical treatments that are common in this course do not exclude the development of conceptual understanding, but without a dedicated measurement, it is difficult to determine with fidelity.

Another component of the design for this instrument was to be of short duration for students to take and for instructors to score. Thus, while open response versions of the items included in this instrument may be very illuminating, the time it takes to assess student understanding in this assessment format is a disincentive to the use of a diagnostic instrument for assessing conceptual understanding. Thus, from the outset, this QCCI was designed as a multiple-choice instrument. The literature on student misconceptions described in the Introduction provided a significant amount of information on how such items could be devised.

An initial pilot version of the QCCI was prepared and edited with the input of professors and postdoctoral students. The initial 12-item instrument was used with a small group from the target audience: undergraduates in a physical chemistry course. Results from the preliminary instrument prompted some minor language adjustments and the addition of two items relating to spectroscopy.

A second version of the QCCI, containing 14 items, was presented to students from various universities and varying class sizes. The topics covered by these items include:

(Item 1) Orbitals (molecular versus atomic orbitals)
(Item 2) Approximations used to simplify many electron systems
(Items 3, 4, 6) Nature of bonding
(Item 5) Correspondence principle—classical limit
(Item 7) Wave nature of particles
(Item 8) Effect of anharmonicity on energy levels
(Item 9) Potential energy curve
(Items 10, 12) Characteristics of a wave function
(Item 11) Qualitative description of quantum mechanical phenomena
(Item 13) Spectroscopy
(Item 14) Wave nature of particles (included in the QCCI that is provided in the Supporting Information but excluded from the analysis presented here; please see the text)

The items fit into the traditionally covered topics. Items 1, 3, 4, 6, and 9 fit into the material relating to molecular orbital theory. Item 2 is traditionally covered during the description of many-electron atoms and molecules and the use of the Hartree−Fock approach. The correspondence principal, item 5, is typically introduced during particle in a box or in the
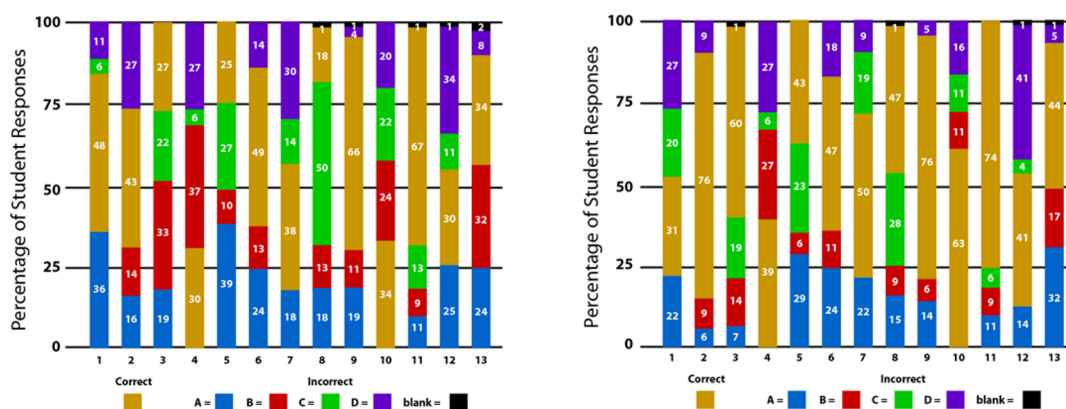
Figure 1. Student responses as a percentage choosing each answer. The pretest (left) includes responses from 166 students, and post-test (right) includes 140 student responses. The correct answer is gold in color in each case. Incorrect answers retain the same color in both graphs, and blank answers are indicated in black.

harmonic oscillator section. The wave nature of particles, covered in items 7 and 14, can fall into several categories but is typically introduced during the treatment of particle in a box. The characteristics of a wave function, items 10 and 12, are introduced in the development of the Schrödinger equation and its solution when discussing the various models such as particle in a box, harmonic oscillator, rigid rotor, and the hydrogen atom. Item 11 is typically introduced early in the course when describing the failure of classical and Bohr models to describe observed phenomena and later in the course when spin and multielectron atoms are discussed. Items 8 and 13 are designed to probe the understanding of quantized energy levels and spectroscopy.

The instrument was used as both a pretest, in the first week of the course, and a post-test during the last week of the course to determine if it was capable of measuring learning gains that resulted from the instruction. The test was administered via Qualtrics online survey program without a time limit. On average, students took approximately 15 min to complete the 14 item revised QCCI. To match student responses from the pretest and post-test, each instructor was given a list of codes to assign to their students. After the final collection, instructors were provided a list of codes for participants who participated in the pretest or the post-test so that participation credit could be given. In exchange for testing the QCCI in their classrooms, professors received a summary report of student responses after both the pretest and post-test implementations of the QCCI. However, none of the instructors reported using the pretest data to explicitly address shortcomings on the instructor survey about their experience with the instrument. A final version of the QCCI can be found in the Supporting Information with the clarification and modification of question 14 from the second version of the QCCI as discussed further in the conclusions and future work.

■ RESULTS

Diagnostic instruments such as the proposed QCCI are useful only if they provide valid and reliable results. This holds true not only for the development, but also for any subsequent usage of the instrument.[39] For an upper-level course, such as physical chemistry, achieving large data sets typically requires several semesters. After favorable results from an initial 12-item trial with 56 students, a second 14-item QCCI was produced. Because of a wording error on one of the distractors, item 14

on the second version of the QCCI had arguably two answers. As a result, all of the results summarized here will be presented on only the 13 remaining items. The items in the second version of the QCCI were offered to nine professors at eight different universities. The universities where the QCCI was given ranged in overall size from roughly 2300 students to over 35,000 students. While seven of the schools (three private, four public) were within the United States, one instructor was at a large Canadian public university. Of the 183 students who participated in using the updated QCCI, 166 took the pretest, and 140 took the post-test. Thus, the student performances used in this analysis included participants from a range of programs. The results presented here provide insight into the psychometric characteristic of the instrument and suggest that it is capable of measuring gains in conceptual understanding that arise from instruction in quantum chemistry.

Pretest and Post-test Analysis

The first set of data for evaluating the performance of the instrument is the breakdown of the student answers in both a pretest and post-test by the percent of distractors chosen (Figure 1). Several observations are worth noting from these data. First, in the pretest administration, all but five of the distractors (1C, 4C, 9D, 11B, 13D) attracted 10% or more of the students, whereas that number decreased by eight in the post-test. The fewer attractive distractors in the post-test indicate that students are better able to avoid misconceptions after a semester of instruction. Second, pretest result from Item 8 performed "below guessing," with less than 25% of correct responses, as might be expected for random answers, but at least a plurality of students chose the correct response in the post-test. These two observations suggest that direct instruction results in a marked improvement in student conceptual understanding.

After instruction, the distractors in Item 1 become more compelling with several students choosing distractors C and D over the correct response, B. Item 1 relates to the relationship of orbitals and electron probability. In general chemistry, the concepts of atomic orbitals (and in some classrooms molecular orbitals) are introduced as a definition—essentially declarative knowledge that students tend to memorize. In quantum chemistry, this definition is expanded and routinely includes information about the mathematical origin of the concept. Given prior research that shows how students focus on mathematical aspects of quantum chemistry,[38] it may be that
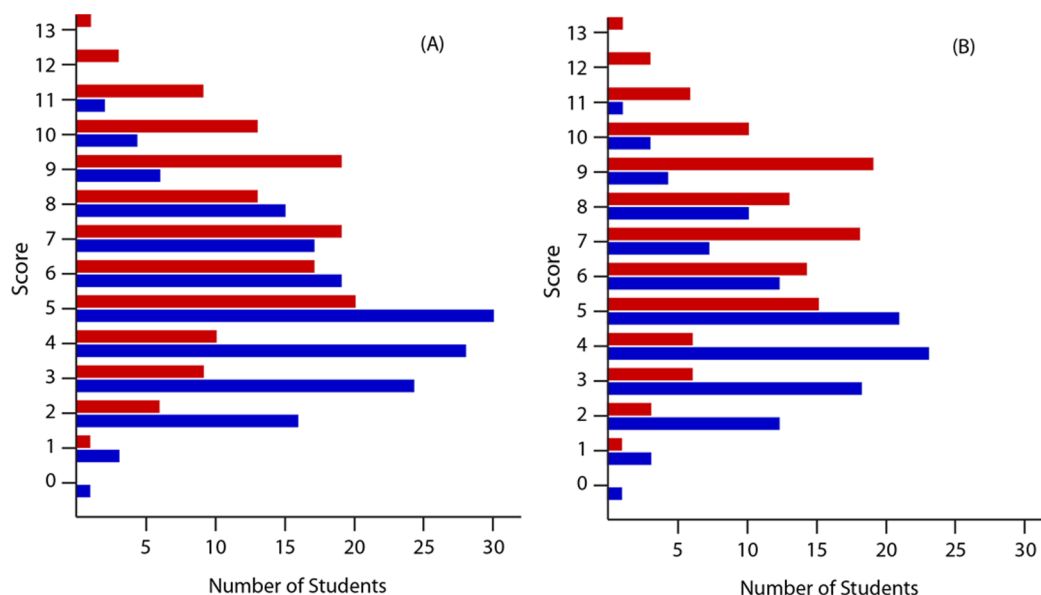
Figure 2. (A) A breakdown of the scores from all students (pretest, 166; post-test, 140) who participated in the QCCI. (B) The breakdown of scores from the subset of students who participated in both pre- and post-tests (115). On the bottom, blue are the performance on the pretest, and the bottom red are the performance on the post-test.

the prior knowledge of concepts and language such as atomic and molecular orbitals become less trusted. Therefore, it may be telling that students exposed to more rigorous mathematical treatments tend to choose more complex responses even though they are incorrect.

A final observation involves the analysis of which distractors students chose. For example, on six items (1, 4, 5, 8, 12, and 13), the performance on the post-test includes distractors that are chosen by more than 25% of students. This last observation alludes to an important conclusion: a semester of instruction does not completely dispel some students' misconceptions or lack of original understanding.

Total Score Analysis

A key challenge in devising a concept inventory that can be quickly administered and scored is devising multiple-choice items that capture student understandings. The ability of the multiple-choice item format to elicit these student misunderstandings is strongly dependent on having good distractors, and this is often the most challenging aspect of concept inventory development.[40] A set of items with relatively few "non-performing" distractors strongly indicates that the QCCI is accomplishing the goal of eliciting student misconceptions within the multiple-choice format. Finally, and perhaps most importantly, this instrument appears to have the desirable characteristic of being able to measure student gains of conceptual understanding in a course that has a significantly mathematical treatment of the science.

Figure 2 provides a learning gain perspective from the lens of student scores on the instrument as a whole. The clear advance in higher scores as a result of direct instruction is not surprising. The important observation to note, however, is that the instrument appears to assess a range of student conceptual understanding in both administrations. In other words, the QCCI maintains it sensitivity to variations in student conceptual understanding both prior to instruction, when misconceptions remain unchallenged, and after a semester of instruction. An instrument that demonstrates substantial

kurtosis in either of these implementations would provide less diagnostic utility as a formative assessment instrument.

Classical test theory can be used to further understand the performance of the QCCI by evaluating the reliability and discriminatory power of the instrument. The range, mean, and median scores are summarized in Table 1. Out of the 166

Table 1. QCCI Scores from All the Students Who Took the Pretest, All Students Who Took the Post-test, and for the Students Who Took Both Pre- and Post-tests

Description	Students, N	Score Range out of 13	Mean Score	Median Score
Pretest Scores				
All students who took pretest	166	0−11	5.1 ± 2.2	5
Students who took both pre- and post-tests	115	0−11	4.47 ± 2.3	4
Post-test Scores				
All students who took post-test	140	1−13	6.9 ± 2.7	7
Students who took both pre- and post-tests	115	1−13	7.2 ± 2.5	7

students completing the pretest, the scores ranged from 0−11 out of 13 points possible, with a mean score of 5.1 ± 2.2 and median score of 5 points. The subset of 115 students who completed both pre- and post-tests were representative of the larger set with scores ranging from 0−11, a mean score of 4.7 ± 2.3 and a median score of 4 points. In the post-test implementation, with 140 participants, the scores ranged from 1−13, with a mean score of 6.9 ± 2.7 and a median score of 7 points. Again, the subset of post-test results from students who completed both the pre- and post-tests was representative of the larger set with scores ranging from 1−13, a mean score of 7.2 ± 2.5, and a median score of 7 points. The Wilcoxon signed ranks test showed a significant difference ($p < 0.0001$) between the pretest and post-test scores of the 115

students who took both with students scoring higher on the post-test than on the pretest. This further supports the sensitivity of the QCCI in being able to detect some changes in students' understanding as they learned quantum chemistry in the semester-long course.

Ferguson's delta (δ) measures the breadth of the distribution of students' total scores over the possible range.[41] In general, tests with a broader distribution of scores tend to be better at discriminating between students at varying levels of understanding.[42] Tests with a δ greater than 0.9 are generally accepted as providing good discrimination among students' understanding. Implemented as either a pre- or a post-test, the QCCI showed acceptable Ferguson's delta values ($\delta_{pre} = 0.94$, $N = 166$; $\delta_{post} = 0.96$, $N = 140$), thus indicating that the QCCI can distinguish students' understanding across the full range of scores. This further supports that the QCCI was capable of discriminating between different levels of student understanding and that the floor effect (a lot of scores close to the lowest score) and the ceiling effect (a lot of scores close to the highest score) were not present in the data collected with the QCCI on either the pretest or the post-test.

Individual item performance was evaluated by comparing item difficulty and point biserial correlation coefficients for each question and for each implementation of the instrument and pre- and post- course instruction. Item difficulty (P) is the ratio of the students who answered the item correctly and the total number of students tested; for example, an item difficulty of 0.8 means that 80% of the respondents answered the item correctly. Items with $P > 0.8$ are typically considered easy, while items with $P < 0.3$ are considered difficult. The point biserial correlation coefficient (r_{pbi}) is used to identify correlations between the students' dichotomous score on an item and their total score on the instrument.[39] The r_{pbi} can indicate whether a particular item can discriminate between high and low performing students, where performance is gauged by their score on the instrument as a whole. For example, an item with a low r_{pbi} indicates that a student's score on that item is not correlated with the student's score on the instrument. Kline defined a satisfactory r_{pbi} as being equal to or greater than 0.2.[43] An item with a low r_{pbi} value could result from the item being misinterpreted, measuring a construct inconsistent with the other items in the instrument, or testing for content that the students have not learned.

Figure 3 represents the relationship between the item difficulty and the point biserial correlation, similar to difficulty and discrimination plots previously described by Luxford and Bretz.[24] Items that are difficult ($P < 0.3$) are expected to have relatively low r_{pbi} values due to a small number of students answering the item correctly. Items considered easy ($P > 0.8$) also could have relatively low r_{pbi} values due to a high number of students responding correctly to those items.

Overall, item performance on only one item on the pretest (Item 8) had a low correlation to the total scores of the respective exams. The focus of Item 8 is the effect of anharmonicity on the energy levels of the harmonic oscillator, which is typically not covered prior to physical chemistry. Item 8 held some gain in the post-test, 0.37 in Table 2; however, it appeared that some students still struggled with the concept.

Normalized Gains Analysis

Normalized gains[44] were calculated for each item to look at the changes in student performance between the pretest and post-test (Table 2). Only the students who were confirmed to have
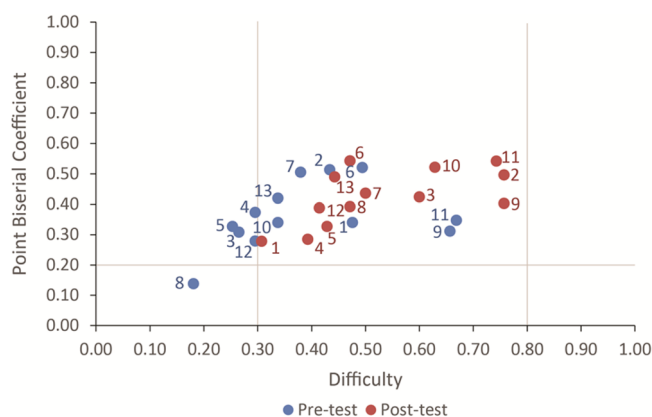

Figure 3. Item difficulty and point biserial correlation coefficients on the QCCI for both the pretest ($N = 166$) and the post-test ($N = 140$) student data. Items with $p > 0.8$ are considered easy items, while items with $p < 0.3$ are considered difficult items. Items with $r_{pbi} \geq 0.2$ are items where the individual item performance correlates with the overall total score for each student.

Table 2. Normalized Gains of the 13 Items on the QCCI for the 115 Students Who Took Both the Pretest at the Beginning of the Course and the Post-test at the End of the Course

Item	Content	Normalized Gain
1[a]	Orbitals	−0.18
6[b]	Nature of bonding	0.15
4[b]	Nature of bonding	0.17
13[c]	Energy levels and spectroscopy	0.18
12	Characteristics of a wave function	0.24
7[a]	Wave nature of particles	0.25
5	Correspondence principle—classical limit	0.27
9	Potential energy curve	0.37
8[c]	Harmonic oscillator	0.37
11[a,c]	Qualitative description of quantum mechanical phenomena	0.38
10	Characteristics of a wave function	0.45
3	Nature of bonding	0.50
2	Approximations used to simplify many electron systems	0.57

[a]Some professors responded that this had been covered in previous classes. [b]The majority of professors responded that students had covered the concepts in this item previously. [c]One professor responded that this concept was *not* covered in their course.

taken both pre- and post-tests were included in the normalized gains calculation. Note that because this instrument was used in several classrooms, and some instructors do not explicitly cover all of the concepts included on the QCCI. All of the concepts, however, were included by a majority of the instructors in the courses they taught. Overall, students performed better on the QCCI after instruction in the course. Item 1, which refers to the relationship between atomic versus molecular orbitals, was the only item where overall the students did worse on the post-test than they did on the pretest. The language used in the distractors, which include phrases typically first encountered in advanced physical chemistry, such as "analytic solutions" and "AOs are derived from hydrogen", appear more favorable to students after the course. While the reason cannot be rigorously deduced without interviews, one can see that, in the pretest, the plurality of students choose between the correct response and

one distractor (Figure 1a, Item 1), whereas in the post-test, student responses are distributed almost equally among the distractors with only a slight plurality choosing the correct response (Figure 1b, Item 1).

Not surprisingly, the largest gains occurred with items that are typically first addressed in advanced chemistry classes: mathematical treatments of quantum systems (Item 2), chemical bonds resulting from fewer than two electrons (Item 3), and wave functions (Item 10). Modest gains are observed in items 5, 7, 8, 9, 11, and 12, which cover common topics in advanced physical chemistry courses. Of these, items relating to spectroscopy and the wave nature of particles include concepts that are often explained, at least conceptually, in general chemistry courses. Item 12 tests the understanding of the mathematical description of a wave function thus depending mainly on a student's understanding of math and may explain the modest gains score. Another explanation for the modest gain can be found by looking at the percentage of students attracted to the incorrect answer choice 12D. After instruction, 40% of the students select "the full wave function can be written as a linear combination of single variable functions". In the pretest, 39% of the students selected 12D. While the correct answer did gain popularity, it seems that answer choice 12D retained its attractiveness even after instruction at the physical chemistry level of rigor.

The lowest non-negative gains scores come from Items 4 and 6 and relate to the concept of bond formation leading to the release of energy, a concept typically covered in introductory courses. The QCCI pretest and post-test data support the notion that students in more advanced courses retain misconceptions from introductory courses and lend evidence toward the persistence of these misconceptions as students gain additional knowledge. The lower gain scores for these items suggest that even for students at an advanced level, this misconception is as robust as has been found with introductory level students.[13,17]

As is true for any concept inventory instrument, the individual item responses are designed to reveal which misconceptions attract students. In this case, it is possible to assess these choices prior to instruction as well as those that continue to attract students after instruction. Because on the QCCI, all of the incorrect answer choices were developed from misconceptions that were previously identified in the literature, an analysis of the student choices can provide interesting information about the relative tenacity with which they seem to hold these misconceptions. Prior work on elucidating student misconceptions has addressed the somewhat arbitrary definition about persistence by indicating that they are important when they are held by at least 10% of the students.[24,45−47] Caleon and Subramaniam[46] suggested additional levels of misconceptions indicating that a misconception that is held by 10% above random chance (i.e., 35% of the students) should be considered significant. Thus, without arguing the relative merits of these different categories, a common misconception may be identified by item distractors that are chosen by 10−35% of the students, and a significant misconception is identified when over 35% of the students choose that particular distractor. The post-test misconceptions measured by the QCCI are reported in Table 3. Examination of these post-test misconceptions may be useful for instructors to devise additional instruction to clarify these issues.

Perhaps just as important as the existence of certain common misconceptions within a sample of students from several

Table 3. Distractors Identified As Containing Either Common or Significant Misconceptions Resulting from the 140 Participants in the Post-test Administration of the QCCI

Item	Concept	Item Distractors (% Chosen)
1	Orbitals	1A (22), 1C (20), 1D (27)
2	Approximations used to simplify many electron systems	—[a]
3	Nature of bonding	3B (14), 3C (19)
4	Nature of bonding	4B (27), 4D (27)
5	Correspondence principle—classical limit	5A (29), 5C (23)
6	Nature of bonding	6A (24), 6B (11), 6D (18)
7	Wave nature of particles	7A (22), 7C (19)
8	Harmonic oscillator	8A (15), 8C (28)
9	Potential energy curve	9A (14)
10	Characteristics of a wave function	10B (11), 10C (11), 10D (16)
11	Qualitative description of quantum mechanical phenomena	11A (11)
12	Characteristics of a wave function	12A (14), 12D (41)[b]
13	Energy levels and spectroscopy	13A (32), 13B (17)

[a]No distractors had 10% or more for this item on the post-test. [b]This distractor was chosen as frequently as the correct response and is the only distractor above 35%, indicating a significant misconception.

universities in the U.S. and Canada, specific trends might merit attention. For example, while Item 1 showed negative gain among the paired pre- and post-populations, the changes in distractor choice are also quite interesting. Initially, students were drawn to a distractor that emphasizes a somewhat simplified view of bonding that students may construct in more introductory exposures. The post-test distractors that become important are those that seem to emphasize mathematical operations of quantum mechanics. Thus, the changes that arise for this item with negative gain for students in introductory quantum courses are consistent with the previously observed behavior[38] that the key to success in quantum classes involves learning to apply mathematical principles.

Other interesting insights arise from considering distractors for which student responses change relatively little in the pre- and post-test implementation. On Item 4, roughly a quarter of students retain the idea that specific information about the identity of atoms involved in a bond influences whether bond formation releases or absorbs energy. Item 12 suggests the concept of a linear combination remains a powerful distractor for students (roughly 40% of students in both the pre- and post-test choose this answer) even as the number of students getting the correct answer increases. Finally, on Item 13, the distractor, where the transition energies are in the opposite of the correct order, actually gains slightly in attractiveness in moving from pre- to post-test. This observation suggests there may be interesting student constructs emerging related to the nomenclature of the wavenumber being cm^{-1}. Follow-up qualitative studies might reveal whether students are somehow inverting these expressions so that large numbers are thought to be small because the unit is suggesting to them the whole value is somehow "in the denominator".

■ FUTURE WORK AND SUMMARY

This paper presents a compact, 14-item concept inventory, dubbed the QCCI, to assess conceptual understanding of key topics of quantum chemistry that are taught in advanced

physical chemistry. The design of the QCCI is meant to provide a tool that requires modest use of class time and is easily graded so it also uses little instructor time to administer. The items in the QCCI were designed based on previously published literature reports about student misconceptions from both chemistry and physics education research as well as general course content.

There are always possibilities to expand concept-inventories because curricular change may emphasize new topics and deemphasize others. The idea that tools such as the QCCI are short so that they require modest amounts of instructional time represents a choice that has implications for the extent of the content domain covered by the inventory: in this case, junior-level quantum chemistry. There are certainly additional topics that could merit inclusion in future editions of the QCCI, but it is important to recognize the value of parsimony in making choices about additions and subtractions. One addition that is anticipated for the next version of the QCCI is to add back in the item on wave properties that had an error in the testing phase. The proposed question has been included in the QCCI, which can be found in the Supporting Information.

When considering the development of new items for a concept inventory, the ability to pose useful distractors is arguably the greatest challenge faced. In the case of the QCCI, the multiple-choice distractors devised from the literature appear to be capable of eliciting misconceptions from students who are at a relatively advanced stage in the chemistry curriculum. It is also important to note that in both pretest and post-test usage, the instrument is capable of determining the variability of understanding in a cohort of students for both test administrations. That is, the QCCI has not shown either a floor-effect or a ceiling-effect in its usage. Finally, the result of direct instruction in quantum chemistry is well reflected in the increase in student conceptual understanding in the course. Thus, even in a course that includes a fair amount of mathematics instruction and mathematical treatments of physical chemistry content, the QCCI provides a means to measure concomitant development of conceptual understanding.

■ ASSOCIATED CONTENT

ⓢ Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00781.

Full QCCI instrument, including the proposed 14th item (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

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