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Representational Transformation and Evidence Chain Construction in Spectroscopic Analysis Instruction

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Abstract: Spectroscopic analysis has been considered a challenging course due to its heavy content, high memorization requirement, and extensive repetition. Recent educational studies indicate, however, that the difficulty does not lie solely in the quantity of information but also in the failure of most students to develop an adequate cognitive schema with spectra. For novices, spectra are often viewed as peak, numerical, and tabular collections; for experienced learners, spectra operate as a multiple representation system that needs to be deciphered based on molecular configuration, bonding environment, experimental setup, discipline-specific vocabulary, and argumentation in science. Educational studies have found that the learning of infrared and nuclear magnetic resonance spectroscopies can be hindered by local cue dependency, dysfunctional chemical reasoning, heuristic manipulation, faulty conceptual model, and fragmented reading strategy. Meanwhile, more competent learners are characterized by spectral comparison, multivariate reasoning, and iterative data interpretation. The development of visualization software, interactive digital tools, real-world data set, spectral puzzle, group work activity, gamification exercise, concept diagnostic test, and pedagogical content knowledge of instructors have provided new perspectives for spectroscopic analysis instruction. Based on this research base, the current study proposes that spectroscopic analysis should not merely be taught through a series of analytical methods and practices but as integrated instruction in representational transformation, evidence chain construction, and academic communication, with particular attention paid to visualization scaffolding, authentic assignment, formative evaluation, instructor knowledge, and equity in education.

1. Introduction

In the past decade, the orientation of research on spectroscopy instruction in chemical education has shown significant changes. In previous years, most articles on the teaching practice mainly concentrated on how to explain an instrument technique well or on providing more exercises. However, the newer literature asks different questions. Specifically, what clues will students follow in interpreting a spectrum? Why can students still fail to make reasonable decisions even though they remember all the typical signals and the rules? The orientation of such research no longer focuses on content itself but moves into the level of thinking mechanism of students during interpretation. Researchers in different aspects of spectroscopic analysis courses such as infrared spectroscopy, nuclear magnetic resonance spectroscopy, mass spectrometry, and ultraviolet-visible spectroscopy have applied methods like eye tracking, retrospective interviews, conceptual instrumentation, error analysis, task design, and the exploration of teachers' pedagogical content knowledge to investigate students' cognitive process. Contrary to people's impression about the fact that such courses are difficult simply because they contain too much information, the above studies reveal a more crucial issue-the main problem facing spectroscopic analysis course is that most students have not learned to read, compare, judge, and discuss about spectroscopic information using the discipline-specific perspective. Viewing from this perspective, a spectroscopic analysis course cannot be viewed as merely knowledge of spectra but should be considered the ground of training to transform among representations. Students are required not to learn just some signals on the graph. Instead, they need to shift from structural formulas, functional groups, electronic environment, vibration mode, fragmentation sequence, oral explanation, experimental background, and decision making. In the lack of proper teaching practice, students will tend to learn spectroscopy only through memorizing and searching information from tables. For example, once students find a characteristic area on the spectrum, they try to decide which functional group the signal corresponds to; once they find the splitting pattern on the NMR graph, they directly apply one of the rules memorized; once they recognize the molecular ion peak, they draw conclusions without considering other clues provided by various spectra. In such a learning procedure, what students obtain is only local proficiency but not the ability to form a reasonable judgement about the spectrum. From the perspective of recent researches analyzing students' activities in spectroscopic tasks, such a gap has been revealed. That is why the current paper does not start from familiar questions like whether the course should be further compressed and online learning platform should be included. Instead, another way of thinking on spectroscopic analysis instruction is adopted. Once the cultivation of students' ability to shift among representations, organize chains of evidence based on incomplete information, and make judgment on the condition of uncertainty becomes the aim of a spectroscopic analysis course, then course content, instructional tasks, classroom discussion, assessment strategies, and teacher roles all need to be changed accordingly. Such a perspective deviates from conventional methods which pay attention to the completeness of knowledge system and innovative methods that solely depend on formal change of courses. It turns back to the most fundamental issue in learning from spectra, namely, have students learned to view a spectrum with a chemist's eye?

2. Discussion of Course Exploration

2.1. Reconceptualizing Spectroscopic Learning in Terms of Representational Transformation

A considerable amount of literature indicates that one of the biggest challenges in spectroscopic analysis is not that learners do not understand particular concepts at all, but that they fail to relate representations of different levels. For example, while some learners may understand that infrared spectra are not just images and that molecules are not merely structures but are actually able to react to the injection of energy, others do not possess that knowledge at all. Moreover, even those who manage to memorize absorption ranges successfully are unable to explain the relationship between peak position and intensity. Thus, based on the above data, researchers argue that the organization of infrared spectroscopy lessons should be focused not on absorption tables but on the conceptual perspective that includes energy, vibrations, and molecule structure. It should be noted that not memorized information, but the ability of students to analyze and compare spectra, to take into consideration several variables, and to produce directed mappings from spectra images to the molecule structure defines successful learners.

As far as NMR is concerned, the same tendency may be observed even more vividly. In the course of experiments dedicated to the examination of proton NMR, novices were found to be concentrated on individual features such as what the particular splitting pattern stands for and what usually exists in the specific chemical shifts. However, experts tended to combine experimental variables, implicit variables, relationships among the peaks, and the possibility of the specific structure altogether. Besides, when discussing the development of expertise in NMR, researchers came to the conclusion that spectral interpretation was not one skill but a set of interrelated domains of knowledge. As a result, the problem of unsuccessful learning did not lie in the incapability of novice students to identify peaks, but in the absence of some kind of bridge for shifting from signal recognition to relational inference. This indicates that a spectroscopy analysis course should be structured not according to the division of content by techniques, but according to the principle of representational transformation between structural formulas, symbolic language, spectrum patterns, oral explanation, and writing. When such transformation is explicitly addressed during the lessons, the ability to move beyond seeing the peaks and coming to a conclusion will turn into an approach that allows learners to narrow the interpretative space progressively via representational transformation. It means that not only should the decision about the choice of techniques used in the analysis be made but also the question of what transformation of representations should be practiced by the students. For instance, the main objective in the case of infrared spectroscopy should not be only in identifying the presence of a carbonyl peak but in explaining how the structure of bonds shapes the vibrational mode, which reflects in the position of the peak. The same applies to the NMR course in that learners should be encouraged not only to identify splitting patterns but also to reconstruct the constraints of neighboring relationships in terms of overall molecule connectivity. Finally, in relation to mass spectrometry, learners should not just memorize rules of fragmentation but trace how ion fragments retain and lose information. Thus, the organization of instruction in the context of these representational transformations may result in more complex understanding of the issue that can be transferred easily.

2.2. Structuring Spectral Interpretation in Terms of Evidence Chain Rather Than Answer Matching

Recent research findings indicate that spectral interpretation is not just a process of answer matching, but a type of evidence-based reasoning. Eye-tracking and interview results obtained during infrared and proton NMR experiments show that learners fail not because they miss some key pieces of information but because they apply some inadequate chemical assumptions or rigid heuristics [1]. To be more precise, learners tend either to accept a single local piece of information too early or reject some information which contradicts the interpretation. That means that the main challenge of the students is the inability to handle relationships among peaks. On the contrary, more expert learners delay closure, compare several sources of information, and modify their hypotheses according to the new spectral evidence. It means that when the instruction is focused exclusively on fast signal recognition, learners acquire the habit of conducting local searches, and they fail to learn how to organize evidence chains. One of the latest findings in relation to this topic refers to infrared interpretation among senior undergraduates and graduate students. It is important to note that the necessity of organizing evidence requires not just reading of the data, but constructing the whole framework which makes it meaningful. At the same time, a good instructor not only provides the right answer, but models how to proceed between the data and interpretative framework. These results have significant pedagogical implications.

For a very long time, "worked examples" in spectroscopic instruction courses were perceived as efficient demonstration of a standard solution of the task by the instructor. However, the most valuable thing that should be demonstrated to students is not the speed of problem-solving or fluency but how to preserve uncertainty, compare two possible interpretations, and modify or refuse the first hypothesis according to the new evidence. Thus, if instructors show the right answers, learners will see only the result. On the contrary, if teachers model hesitation, elimination, returning to the initial solution, revision, and reorganization, then students will have a chance to understand the process behind the solution. This means that the structure of tasks performed in class should shift gradually from single-answer tasks to those related to evidential sufficiency, conflicting information, and uncertainty. For example, instead of repeatedly asking students to find the match between a typical spectrum and a structure, learners may be required to compare two similar infrared spectra and identify the difference that may become diagnostic. Instead of requiring to write down the structure, learners should be offered to determine which spectral feature is most helpful, which is the least relevant, and what other evidence could be collected if there were another set of data. Such tasks are not more complicated than the previous ones but they better illustrate the way of judgment in chemical practice.

2.3. Transforming Invisible Processes into Visible Ones Through Visual and Interactive Scaffolding

One of the major challenges of spectroscopic analysis consists in the inability of learners to relate spectral signals to molecular behavior. In terms of infrared instruction, researchers managed to create interactive web-based environments, physical models, and inquiry tasks that allow students to combine vibrational modes, functional group motion, and spectral changes [2,3]. Such approaches are beneficial not because they make the lessons more contemporary and visual but because they enable conversion of the invisible processes that can be illustrated only in verbal forms into manipulative ones. In relation to NMR, digital tools, web-based practice programs, and visualization technologies are effective not because they present learners with additional problems but because they help in establishing continuous mappings between chemical shift, integration, splitting, and structural environment. One of the peculiarities of such scaffolding is that learners tend to externalize their thinking through these technologies. Thus, whether it is open-source spectral games, online NMR practice programs, jigsaw tasks, tabletop games, or escape room-type activities, the real value of them is in the ability to transform implicit judgments of students into visible actions that can be further analysed by their colleagues. On the contrary, digital tools which simply transfer the questions to the screen and provide learners with instant feedback do not allow them to think but just perform tasks faster. Therefore, the usage of visual and interactive support in spectroscopy lessons should be based on one crucial premise-technology should make the process of judgment more visible for the learners, but not make the judgments for them. Visual scaffolding calls attention to another important issue-that of accessibility of spectroscopy instruction. Some studies tried to convert infrared spectra into auditory presentations to ensure visually impaired people could analyse peak patterns and frequencies. Other researchers raise the question whether it is possible to conduct spectroscopy lessons avoiding visual matching that results from the image-search era. While initially this problem may seem marginal, it is important to note that spectroscopic analysis is not a subject where only one visual pathway leads to the result, nor is it a set of lessons where memorization of patterns guarantees success.

2.4. From Example-Based Exercises to Real Analysis Problems

The reason why students complain that they "can solve the problem but cannot analyse" lies in the heavily templated nature of classroom examples. Spectra are nice, information is perfect, hints are obvious, and problem types are familiar. Instead of learning how to think, students learn how to detect the pattern of an expected answer. In the past few years, more research on education has sought to incorporate authentic or quasi-authentic data back into the instruction. Some studies offer students curated multispectral data sets suitable for undergraduate use. Others create unknown puzzles based on experimental rather than textbook-like spectra. Others develop project-like activities where students are assigned to deal with authentic infrared, NMR, and mass spectrometric data of real-world substances. The common point is the blurring of the distinction between classroom, research, and practice in students' mind. Students are made aware that sometimes real data do not carry sufficient information, and the analyst should know how to work with incomplete, noisy, and redundant information.

However, bringing authenticity does not mean creating a project-like course. Much more fundamentally, it requires a change in the cognitive architecture of the task. Authentic tasks differ from textbook examples at least in three aspects. First, students are not provided with pre-selected information but must determine themselves what information is relevant to the problem at hand. Second, judgments are usually justified using several types of evidence, not a decisive peak alone. Third, besides the ultimate conclusion, students are required to demonstrate the reasoning leading to the answer. As seen in the discussion of research on jigsaw cooperation, spectral puzzle, spectral game, and test design in structural analysis, the teaching focus has gradually moved from "getting the structure" to "justifying how the structure is obtained". This gradual shift demonstrates how the course evolves from knowledge rehearsal towards participation in the practice of chemistry.

On the other hand, authenticity should never be understood as total complexity. Beginners may only become frustrated if they encounter real and complex data without any assistance. The appropriate route should be gradual introduction of authenticity. After students are taught how to choose among possibilities in semi-open tasks, they will learn to analyse information-rich spectra. After dealing with organization of evidence in small molecule cases, they will gradually learn to engage in broader structural interpretations. After mastering local justifications, they will be asked to construct a full chain of reasoning. Authentic tasks do not substitute traditional exercises one-to-one. They require rethinking of task gradients so that students gradually learn how to maintain interpretative control in progressively more complex situations.

2.5. Assessing Student Reasoning Rather Than Correctness of Their Answers

Given the new direction that the spectroscopic analysis course should take, new directions in assessment should follow. Research in recent years has tried to develop a range of assessment tools to address the process of reasoning itself. There exist instruments that assess NMR representational competence. There are concept inventories that evaluate the understanding and interpretation of proton NMR data [4]. There are examinations based on spectrum-puzzle-type problems of structure determination. Finally, there is a study analysing reasoning mistakes committed by students working on a structural analysis. All together, they suggest that traditional correctness-focused assessment often allows us to check only whether students generate an expected answer. The process of reasoning underlying the result may remain invisible, particularly if it results in a correct answer regardless of mistakes in the process. This means that spectroscopic analysis assessment should pay attention to several things besides checking correctness. First, can students move between representations? They should be able to interpret a spectral phenomenon structurally and vice versa. Second, can students justify their answers? In addition to presenting the evidence, they must be able to explain the weight of evidence. Third, can students express uncertainties? In particular, can they say when the available data are not enough for drawing conclusions? Such assessment will not necessarily imply a higher number of questions. However, it will make students pay more attention to justification rather than quick generation of correct answers. They will gradually recognize that a well-supported interpretation is more valuable than the answer itself.

Another interesting aspect is that students do not find all spectroscopic methods equally easy. According to some studies, students perceive IR spectroscopy as relatively easy, while mass spectrometry as the hardest method of all to master. It means that, if the instructor assesses students' work with spectroscopic data in general, s/he will miss method-specific cognitive thresholds. Thus, assessment should not be a mere documentation of learning outcomes. It is supposed to diagnose the problem areas-whether students face difficulties of conceptual understanding, representational transformation, reasoning chains organization, or academic communication. Only when assessment is used as a diagnostic tool, the teaching of spectroscopic analysis can truly focus on learning problems.

2.6. Paying Attention to Teacher Knowledge and Equity in Learning

When the research perspective shifts to cognition, a role of the teacher changes as well. Recent studies on the teaching of proton NMR show that pedagogical content knowledge here is not an ability of a general nature [5]. On the contrary, it can be topic specific and associated with certain subtopics, types of tasks, or even layers of questioning [5]. Additional studies indicate that such knowledge develops through teaching experience. The later research shows how instructors' choice of representations, emphasis on certain concepts, and organization of class discussion play a crucial role for quality courses. In other words, in order to teach spectroscopic analysis better, instructors need not only good books or ample opportunities for practice. They also need knowledge of common student mistakes, critical difficulties in learning, and transitional patterns.

Even the form of discussion may be significant for students' willingness to participate in spectral interpretation. A study conducted in 2025 shows how the same communicative assignment can evoke gender-specific responses depending on its framing: if students are encouraged to evaluate their abilities in NMR communication, they react differently than when exploring people's communicative behaviour [6]. This finding is extremely relevant to spectroscopic analysis because spectral interpretation is a very visible task. Often, it involves public explanation of reasoning, including potential uncertainties and mistakes. Therefore, the classroom discourse culture built upon the hidden norm that the best student is the one who appears to be the most proficient quickly, can silently filter out students unwilling to risk making a mistake. Teaching spectroscopic analysis means not only developing cognitive skills. It also involves creating a safe classroom environment for exploration. For this reason, learning equity should not be seen as something external. On the contrary, class environments that allow for tentative reasoning and discussion without fear of immediate evaluation by instructors may help in giving more students access to the very core of the discipline. When students are allowed to experiment with various explanations and hypotheses without a quick judgment whether the reasoning is expert-like or not, they are more likely to participate actively in the practice of spectral interpretation. Thus, paying attention to teacher knowledge and classroom discourse is not a secondary thing. On the contrary, it becomes a prerequisite for successful teaching.

3. Reflection on Teaching Practice

First, if the above-mentioned ideas are implemented in practice, they are most likely to result in three key changes. First, students' focus will gradually change from identifying features to explaining relationships. While this does not mean that students will become skilled in resolving complicated issues, it means that they will start being interested in the reasons behind which the specific signal proves or disproves a certain hypothesis. Besides, the process of spectra analysis will stop being entirely linear, and will involve repeated moving back and forth between structures and signals.

Finally, classroom discussions will shift their role from checking answers to practicing the process of decision-making, which corresponds to mature interpretation skills advocated in academic literature. With instructors being ready to put reasoning processes rather than only correct answers at the heart of classroom interaction, the process of spectroscopic analysis is bound to develop into something far more profound and relate to academic communication, evidence usage, and responsible judgment. Second, there is another potential risk, though. While introducing innovative formats of the course, many instructors may try to make use of gamification or technological tools, or any other aspects associated with gamification, assuming that they alone guarantee successful teaching. However, the format is less significant than the process of forcing students to go beyond mere matching of features, engage in representational transformations and find ways to organize evidence. Introducing technological tools or a puzzle-solving format as an additional element to the process of resolving problems can only make students more interested and keep them engaged in the same surface activities as before. At the same time, using authentic data without sufficient preparation can make students guess and look for clues in the hope of guessing the right thing. Therefore, when exploring course formats, instructors should think of the way of developing reasoning skills rather than creating a new game. Another factor that needs to be considered while exploring options for the course is the necessity of changing its approach. The more it focuses on reasoning, the more difficult it is to teach spectroscopy using the instructor's own experience. When it comes to diagnosing students' reasoning processes, teachers need to be aware of the assumptions their students often make; identify difficulties associated with certain representational transformations; unpack their experts' reasoning and show uncertainty; and encourage students to develop critical reasoning. For most teachers used to building lessons based on fluency, it is not easy to change one's approach. If the format of professional development programs is focused solely on designing lectures rather than helping teachers diagnose the process of their students' reasoning and give appropriate feedback, any significant changes in the course cannot happen. Third, the issue of equity and accessibility is vital in any course exploration and design. Many instructors believe that spectroscopic analysis is a subject in which "the more intelligent students naturally perform well"; however, according to educational literature, this difference is often determined by whether or not the classroom provides opportunities to express ideas partially; whether mistakes made by students are seen as learning material; and whether students having different levels of expertise receive enough support. If the course evaluates only rapid and correct solutions, many students are going to start resembling "a good spectroscopist" and get higher grades; others will stop participating in discussions and drop out. At the same time, if students are given a chance to make comparisons, reconsider their choices, and discuss things in class, they will learn about spectroscopy as a discipline rather than a natural gift. High quality spectroscopy teaching is not aimed at helping the best students to learn faster; it is meant to provide more students with an opportunity to participate in the process of judgment.

Thinking long term, any course design needs to answer the question of whether the students have started to acquire a stable skill of making chemical judgments. After leaving this course, they are expected to be able to compare spectra to understand them; to recognize the contradictions between the pieces of evidence; to recognize the limitations and the amount of information necessary for making conclusions. As far as the course fulfils these goals, its function as an education course can be considered fulfilled.

4. Conclusions

With the current research on chemistry education, spectroscopic analysis should not be seen as a purely content-oriented subject. However, this does not imply that there is any need for fostering mere passive remembering of characteristic peaks and general principles. On the contrary, such an approach implies the ability of students to navigate actively through structures, spectra, conditions, languages, and judgments related to the subject matter. In this case, it becomes apparent that the critical thing to consider when designing a course on spectroscopic analysis includes not just techniques, resources, and difficulty levels but most importantly, ways to involve students in interpretation of spectra. In other words, the goal is to help students move from recognizing isolated phenomena to establishing relationships among them, from consulting reference tables to developing conceptual understanding, and from guesswork to constructing sound chains of evidence. Such a consideration suggests that there are five possible areas where future research might be concentrated. Firstly, the explicit aim to achieve representational transformation can be established. Secondly, evidence chain formation should remain the core issue discussed in the classroom environment. Thirdly, technology should be used not only to produce new representations but also shed light on implicit cognitive processes. Fourthly, exercises should be scaffolded and based on real-life situations. Lastly, assessment could consider not just answers to questions but more importantly, arguments, comparisons, and communication. It is only through the combined action in all the directions indicated above that spectroscopic analysis might overcome its negative reputation of being an extremely challenging, highly disintegrated, and almost impossible to remember subject. Moreover, it can become a valuable learning activity.

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