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AN OPEN ACCESS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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Perspective

The Complexity of Reasoning about and with Chemical Representations

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Cite This: *JACS Au* 2022, 2, 2658–2669

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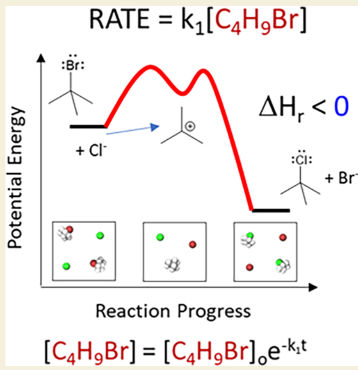
ABSTRACT: External visual representations of chemical entities and processes (chemical representations) play a critical role in chemical thinking and practice. They support reasoning by serving as bridges between the macroscopic world and the chemical models that help us make sense of the properties and behaviors of substances in our surroundings. Consequently, many chemistry education research studies have been carried out to explore and foster students' representational competency in our discipline. Nevertheless, in this Perspective I argue that investigations in this area would benefit from a more in-depth analysis of how the distinctive characteristics of chemical representations affect student reasoning. I identify four dimensions of variation in these representations (iconicity, quantitativeness, granularity, dimensionality) that affect students' ability to interpret, connect, generate, and use chemical representations. I discuss how these features influence the unpacking or packing of information during different types of tasks, affecting sense-making and perceptual competency. Implications for chemistry education research and practice are considered.



KEYWORDS: *Chemistry Education, Chemical Models, Representations, Representational Competency, Student Reasoning*

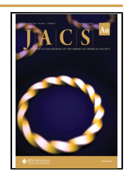
INTRODUCTION

Chemistry education research and practice are intricately linked to the use of external visual representations of chemical entities and processes (hereafter, chemical representations) for communicating concepts and ideas, guiding and supporting reasoning, and fostering understanding.[1−4] Multiple research studies in education have been carried out to gain insights into how students and instructors engage with chemical representations and interpret, connect, generate, and use them while making sense of phenomena, building explanations, making predictions, or constructing arguments.[5−24] Similarly, diverse educational projects have sought to develop and implement a variety of strategies and tools to support chemistry teachers and students in the use of chemical representations during the learning process.[25−32] Overall, significant research and development efforts have been dedicated by the chemistry education community to better support students' acquisition of representational competency[33,34] in our field.

Despite these substantial and impactful efforts, in this Perspective I argue that work in this area would benefit from a more detailed analysis of how the distinctive nature of chemical representations may influence students' reasoning about and with them. Although all natural sciences rely heavily on external visual representations while engaging in their disciplinary practices, each of these sets of representations have domain-specific characteristics[1,35,36] that are important to recognize to better support student reasoning and learning in each area. Thus, the central goal of this essay is to provide a more in-depth look at the nature of chemical representations and discuss how their specific features may interact with student reasoning.

As a chemistry education researcher working in this field for over 20 years, I consider it important to carefully reflect on the nature of chemical knowledge and practice to guide educational research and instruction. The ideas advanced in this paper are based on my personal analyses of the types of chemical representations used in foundational chemistry courses (i.e., general and organic chemistry) in secondary schools and at the college level across the world, informed by major findings from existing research on how students, instructors, and instructional designers engage with and use these types of external visualizations.[37−40] I approached this analysis from the perspective of a researcher interested in novice and expert reasoning in chemistry who has greatly benefitted from work in the area of representational competency in chemistry and other science, technology, engineering, and math (STEM) fields. Nevertheless, my analysis may be biased by the focus of my research and my personal conceptualization of how chemists think.[41,42]

Received: September 12, 2022
Revised: October 25, 2022
Accepted: October 27, 2022
Published: November 9, 2022



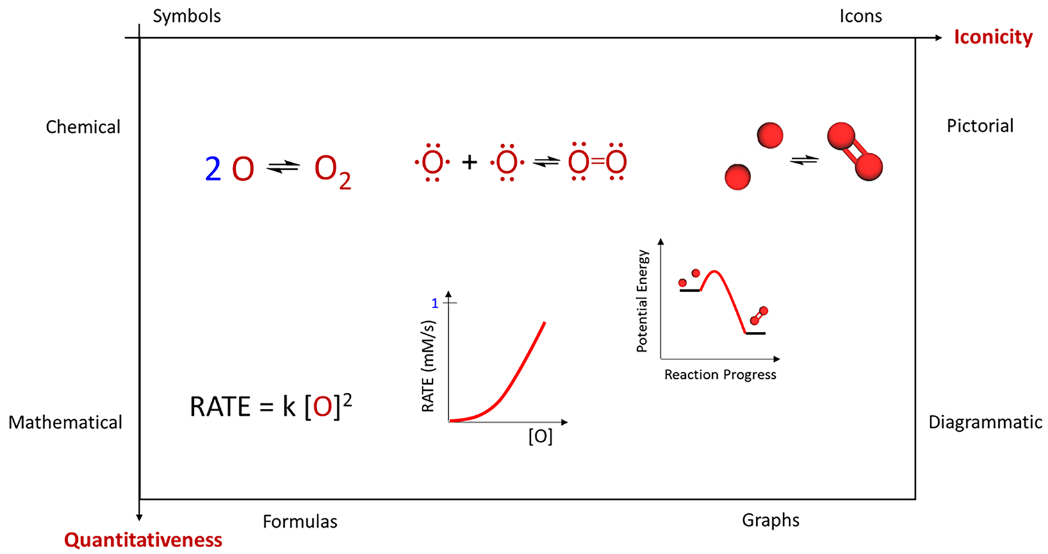


Figure 1. Examples of chemical representations related to the same chemical process but exhibiting variation along the *iconicity* and *quantitativeness* dimensions (these representations also vary in terms of granularity and dimensionality, but these differences are not highlighted in the figure). Chemical symbols and pictorial icons typically provide more explicit qualitative information than mathematical symbols and diagrammatic icons (e.g., graphs).

Dimensions of Variation of Chemical Representations

Different authors have discussed the central role chemical representations play in the thinking and practice of chemistry.[1−4,23,42−44] These representations are not only used to facilitate the communication of concepts or ideas but also to enable reasoning about chemical entities and processes.[43,45] They serve as bridges between the tangible material world we seek to describe, understand, transform, and control and the theoretical principles and models developed by chemists to make sense of the properties and behaviors of substances in our surroundings.[42,44] Although chemical representations are quite varied, I contend that major differences can be noted along the four major dimensions of analysis defined in the following paragraphs:

Iconicity. Chemical representations can be conceptualized as visual signs that communicate information about an object, state, event, or process. These signs may be "symbolic" in the sense that there is an arbitrary connection between the sign and the content it represents, such as the chemical symbols for the chemical elements. Or the signs may be "iconic" in that they exhibit some degree of natural and nonarbitrary relation between sign and content, such as the ball-and-stick pictorial representations of molecules.[45−47] Iconic signs often rely on analogical (e.g., an atom depicted as a small ball) or metaphorical (e.g., a higher peak in an energy diagram is frequently interpreted as a larger energy "barrier") connections to convey meaning. Chemical representations expand the continuum between symbols and icons, exhibiting different degrees of iconicity.[43] Take, for example, Lewis structures or wedge-dash representations of molecules in which symbols for different types of atoms are combined with structural icons that represent atomic connectivity or molecular geometry.

Quantitativeness. Chemical representations may convey explicit qualitative information about the nature and properties of represented entities such as their physical state, chemical composition, or partial charge, but also different degrees of explicit quantitative information in the form of relative value of measurable properties (e.g., composition ratios in chemical formulas, larger vs smaller radii in molecular models, higher vs lower energies in energy diagrams), actual numerical data (e.g., graphs, spectra), or mathematical relationships between variables (e.g., $PV = nRT$).

Granularity. Visual representations in chemistry depict entities or processes at one or multiple granularity levels,[48,49] from the macroscopic to the electronic scales. Each granularity level is characterized by specific objects, such as atoms at the atomic level or electrons at the electronic level, with properties that one seeks to highlight. These properties often emerge[50] from the dynamic interactions of collections of objects at a lower granularity level. For example, interactions between bonded atoms at the atomic level give rise to the molecular geometry of the system at the molecular level; interactions between protons and electrons at the electronic level determine atomic sizes at the atomic level.

Dimensionality. Chemical representations explicitly highlight different properties of targeted entities corresponding to one or more physical or chemical dimensions, including chemical composition, structure (e.g., atomic connectivity, geometry), electrical properties (e.g., charge, polarity), mechanical properties (e.g., interaction forces, potential energy), and kinetic properties (e.g., rate, time).[42,51]

Figures 1 and 2 seek to illustrate variation in chemical representations along the four dimensions of analysis described above. Depicting variation along four different dimensions is difficult, so the figures highlight differences along a pair of selected dimensions. Figure 1 emphasizes variation along the iconicity and quantitativeness continuums using representations linked to the formation of diatomic oxygen from atomic oxygen as examples. This chemical process is represented in the figure using varied visualizations, from a symbolic chemical equation to a more iconic representation of the atoms and molecules involved. These representations explicitly provide qualitative and quantitative information about chemical composition and structure. The level of quantitativeness increases for those representations that convey information about the mathematical relationship between the rate of reaction and the concentration of atomic oxygen in either symbolic or graphical form. In contrast to these latter examples, the energy diagram in Figure 1

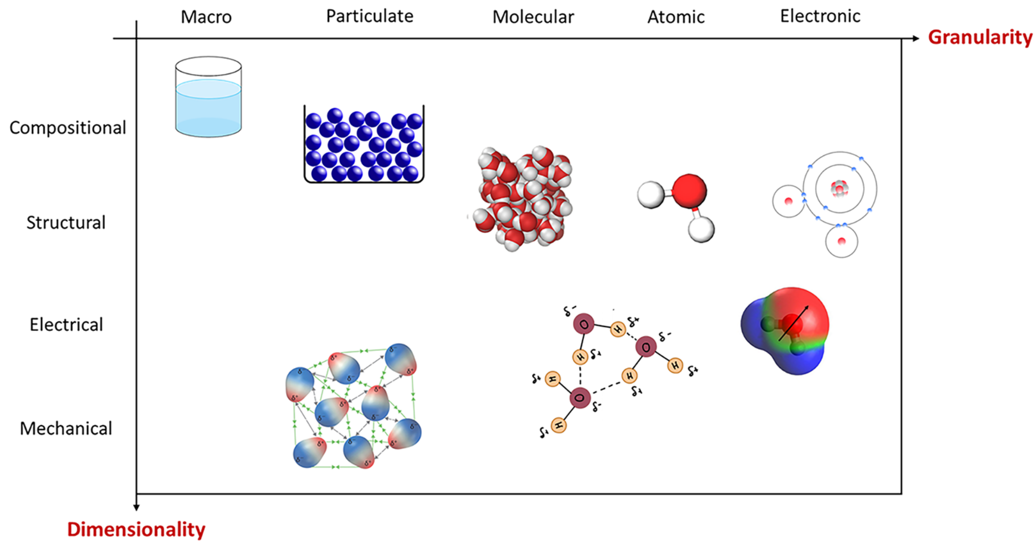


Figure 2. Examples of chemical representations related to the same chemical substance but exhibiting variation along the *granularity* and *dimensionality* dimensions (these representations also exhibit slight variations in iconicity and quantitativeness that are not highlighted in the figure). Representations are placed at the granularity and dimensionality levels they make most explicit although they may include elements from other levels.

exhibits a relatively lower degree of quantitativeness, as it depicts only relative potential energy values (i.e., higher or lower energies) and a greater degree of iconicity in its representation of the activation energy barrier.

Figure 2 includes different chemical representations related to the same chemical substance (water) with slight variations in terms of iconicity and quantitativeness but much larger differences along the granularity and dimensionality axes. Along the granularity axis, each representation makes explicit different components, such as particles, molecules, atoms, and electrons, that are relevant at different scales of analysis. Along the dimensionality axis, representations vary on the types of chemical or physical properties that are made explicit or emphasized, from chemical composition to molecular structure to charge distribution to intermolecular interactions. One can expect some chemical representations to present explicit information about various granularity or dimensionality levels, making it difficult to place them in a multidimensional space. For example, chemical representations that display information in the electrical dimension may include compositional and structural information, and representations at an electronic level of granularity will probably include atomic and molecular elements. However, a given representation is typically used to highlight specific components and properties as illustrated by the electrostatic potential map in Figure 2, which contains explicit structural information but mostly emphasizes the electrical dimension. Thus, the dimensions that characterize a given representation may vary depending on how and for what purpose it is used.

As Figures 1 and 2 illustrate, characterizing differences in chemical representations by just making assignations based on the three categories associated with the well-known chemistry triangle or triplet (macroscopic-symbolic-submicroscopic)[42,44,52,53] does not necessarily capture the richness and complexity of the multiple types of representations with which we expect chemistry students to engage. This approach may conceal the reasoning needed to interpret, connect, generate, and use various types of chemical representations in productive ways in diverse contexts and for different purposes. As discussed in the next section, acknowledging such a complexity is needed to better understand the reasoning challenges that chemical representations pose to chemistry learners and for devising strategies that support the development of representational competency in chemistry.

Interpreting Chemical Representations

The four dimensions of variation of chemical representations defined and described in the previous section point to major aspects or features of a given representation that need to be recognized to properly interpret its meaning. Interpreting a chemical representation demands providing answers to questions such as What types of entities (granularity) and properties (dimensionality) are being represented? What types of qualitative and quantitative information can be directly or indirectly inferred (quantitativeness)? What relevant attributes (explicit or implicit) does the representation convey (iconicity)? Failing to adequately answer any of these questions is likely to result in misinterpretations that will affect reasoning about and with the representation. As illustrated in the next paragraph, examples of reasoning issues resulting from inference errors along the granularity, dimensionality, iconicity, or quantitativeness dimensions are abundant in the chemistry education research literature.

For example, students often fail to differentiate between the symbol H_2O, which refers to a molecular entity, and the symbol $H_2O(l)$, which refers to a macroscopic chemical substance.[22,23] Thinking of the representation $H_2O(l)$ as corresponding to a chemical entity at the molecular rather than the macroscopic levels (granularity issue) may reinforce the intuitive belief that molecules have macro-like properties.[54,55] The same type of intuitive reasoning may be prompted when thinking of the colors used to represent different types of atoms as iconic rather than symbolic cues (iconicity issue).[56] Similarly, assuming that the symbol NaCl corresponds to a molecular rather than an ionic entity (granularity and dimensionality issues) will affect inferences about the structure and properties of the chemical entity to which it refers.[57,58] Considering that the different colors in an electrostatic potential map are indicative of variations in temperature or heat rather than in electric potential (dimensionality issue) will constrain reasoning about inter-

https://doi.org/10.1021/jacsau.2c00498
JACS Au 2022, 2, 2658−2669

molecular interactions.[59] Thinking of reaction progress in an energy diagram as a measure of time rather than conversion progress along a reaction pathway (dimensionality issue) will affect reasoning about relative reaction rates.[60] And taking the symbol 3 H_2 to represent a single molecule with six hydrogen atoms rather than three independent diatomic molecules (granularity and quantitativeness issues) will likely hinder understanding of the changes that take place during a chemical reaction.[61]

Inferring the proper levels of granularity, dimensionality, iconicity, and quantitativeness when engaged with a chemical representation is not easy for novices, particularly when some of the information that the representation conveys is implicit rather than explicit.[12] Even if a large fraction of this information is explicit, one needs to decide which of the represented features are relevant for meaning making.[62] One can expect that the lower the degree of iconicity of a representation, or the more symbol-like it is, the higher the ratio of relevant to irrelevant attributes included in the representation will be, which may decrease the cognitive effort needed to build an interpretation. However, symbolic representations tend to be more abstract than iconic ones, which could hinder sense-making processes.[63] Additionally, the ratio of explicit to implicit relevant features can also be expected to affect reasoning. For example, students are more likely to struggle making inferences about molecular geometry from a molecular formula that has a lower ratio of explicit information, such as atomic composition, to implicit information, such as atomic connectivity and electron domains, than from the associated Lewis structure where these two features are made explicit. These different, and sometimes competing, factors need to be considered when analyzing how students engage with different chemical representations.

Explicit features in a representation are likely to provide information that is aligned with the specific levels of granularity, dimensionality, and quantitativeness of the representation, facilitating reasoning at those levels but not necessarily at others. Consider, for example, the pair of representations of water vapor in Figure 3, which vary in their level of iconicity,

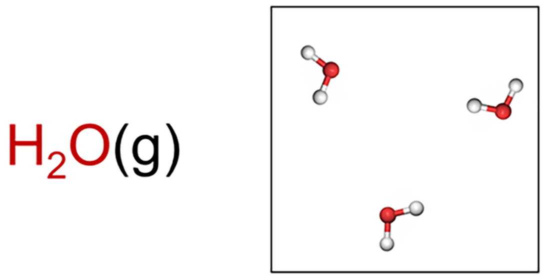


Figure 3. Symbolic and iconic (molecular) representations of water vapor.

granularity, and dimensionality. Most features in the symbolic representation $H_2O(g)$ are explicit and relevant in making inferences about the chemical composition and physical state (dimensionality) of the represented macroscopic substance (granularity). On the other hand, the attributes needed to build the same type of inferences using the molecular representation on the right side in Figure 3 are mostly implicit. One must, for example, infer elemental composition from a color code and state of matter from the relative distance between molecules. Additionally, this more iconic representation includes several features that are irrelevant in making inferences about chemical composition and physical state, such as the number, location, and orientation of the molecules depicted. Inferences about chemical composition are thus likely more easily made using the symbolic representation. However, the molecular representation on the right facilitates the generation of inferences about molecular structure, as this attribute is explicit in this visualization, while extracting information about the molecular nature of water vapor and the atomic connectivity and molecular geometry of its molecules from the symbolic representation $H_2O(g)$ requires a long chain of cognitively demanding inferences built on information tacitly linked to each chemical symbol (e.g., number of valence electrons, relative electronegativity). Student reasoning is thus likely facilitated when information can be directly inferred from explicit features of the representation.[9]

Connecting Chemical Representations

Highly symbolic chemical representations encapsulate information that needs to be unpacked or decompressed to build connections to other representations[28,64] or generate new representations that differ in one or more of the four dimensions highlighted in this work. This "unpacking" demands knowledge of disciplinary conventions, known patterns, classification systems, procedural rules, and modeling primitives that support reasoning about and with chemical representations. I use the term "modeling primitives" to refer to pieces of knowledge in a domain with general applicability that can be reused in the modeling and building of representations of diverse systems.[65] Examples include: the most electronegative atom in a bond tends to acquire a negative partial charge, the formation of chemical bonds releases energy, the mechanistic step with the highest activation energy is rate-limiting.

Chemical representations contain explicit cues, such as the types of atoms present, atomic connectivity, and molecular geometry, that may be used to trigger relevant knowledge, conceptual and procedural, that supports the connection to or constructions of other representations. Consider, for example, the symbolic representation of a water molecule H_2O. This representation conveys explicit compositional information about the molecule that can only be properly extracted if one has knowledge of chemical language conventions (e.g., H represents the element hydrogen) and chemical formula conventions (e.g., subscripts after a symbol indicate number of atoms of that element present). Connecting or translating this representation into a Lewis structure demands recognition of the molecular nature of this entity based on the classification of hydrogen and oxygen as nonmetallic elements, and the modeling primitive that stipulates that the chemical combination of nonmetallic elements is likely to generate molecular compounds. The Lewis structure can then be constructed through the application of procedural rules that require knowledge of periodic patterns.

The process of unpacking a representation may be quite challenging, as it demands the identification of relevant explicit cues that can be used to activate and integrate a variety of pieces of knowledge (conceptual and procedural). Research in chemistry education has shown that students at all educational levels struggle with common unpacking tasks such as differentiating and classifying substances into chemical groups based on representations of their chemical formulas or structures (e.g., differentiating elements, compounds, and mixtures,[66] ionic and molecular compounds,[58] acids and bases,[67] nucleophiles and electrophiles[68]), connecting compositional to structural features

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(e.g., translating chemical formulas into Lewis structures[69]), or inferring electronic properties from structural information (e.g., assigning partial charges based on type of substituents[70]).

Chemical representations can also be packed or compressed to generate representations with lower degrees of iconicity. "Packing" a representation reduces the amount of information that is represented, making the representation more general, denser in relevant features but also more abstract. This process demands recognition of what features should be preserved and how their representation may change to make them more explicit.[62] For example, in moving from the molecular representation to the Lewis structure in Figure 4, chemical symbols become explicit, but bond orientation becomes irrelevant. In compressing the Lewis structure to the chemical formula, explicit information about atomic connectivity is not preserved, and chemical composition information is made explicit.

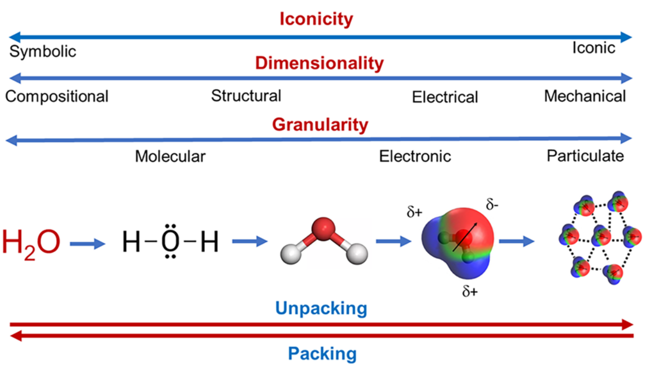

Figure 4. Examples of unpacking and packing of information is a set of chemical representations and their effect on the iconicity, dimensionality, and granularity of the representation. Representations are placed at the granularity and dimensionality levels they make explicit within the sequence of inferences represented in the image (i.e., inferring molecular geometry, charge distribution, and intermolecular forces from molecular composition).

It is through unpacking and packing of information that we change the granularity, dimensionality, iconicity, and quantitativeness of chemical representation as illustrated in Figure 4. Unpacking makes some information explicit often through the inclusion of more symbols or icons whose meaning needs to be understood, such as the use of lines or bars to represent bonds, or the addition of symbols or colors to differentiate positive and negative partial charges. Other information, however, may become implicit as when explicit chemical symbols are replaced by a color-coding scheme that implicitly conveys information about chemical identity. Unpacking takes us from more general symbolic representations to more specific representations with higher iconicity that often include more irrelevant features for purposes of interpretation or translation. This is illustrated in Figures 3 and 4. The representation on the right side of Figure 3, for example, is one of many possible molecular representations that one could link to the general symbolic formula $H_2O(g)$. These molecular representations can vary in terms of number of molecules represented and their orientations, as these features are irrelevant in building inferences about state of matter, chemical composition, or molecular structure. Packing, on the other hand, results in more general and abstract representations with a higher density in relevant attributes.

One could hypothesize that unpacking tasks may be often more cognitively demanding than the packing of a representation. However, existing research suggests that the latter types of tasks can also be challenging, as they demand knowledge about conventions and rules for what information is preserved and how.[14,64,71−75] For example, to translate the ball-and-stick model of water in Figure 4 into the symbolic representation H_2O, one needs to know the color-coding system used to represent different kinds of atoms as well as the conventions for writing chemical formulas. Educational research indicates that students do not necessarily translate more easily from iconic representations identified as submicroscopic or particulate to symbolic ones (which often require packing information) than from symbolic to particulate (which often require unpacking).[10] For instance, many students fail to write the proper chemical equation that corresponds to a chemical reaction represented at the particulate level,[76] while they seem to engage with the reverse process more easily. This is likely related to the implicit nature of the information needed to generate the chemical equation from the particulate representation and to the one-to-many nature of the relationship between a symbolic representation (general) and associated particulate representations (specific) as illustrated in Figure 5 for the synthesis reaction for water.

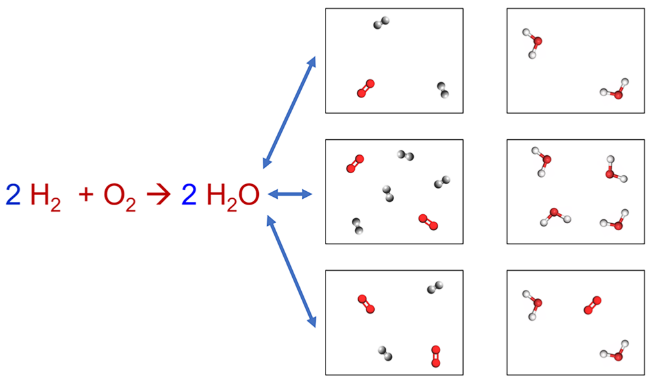

Figure 5. Different iconic-molecular representations associated with the symbolic-molecular representation (chemical equation) for the synthesis reaction for water.

The translation from symbolic to iconic in Figure 5 can be done by building direct associations between symbols of reactants and products and their associated icons (e.g., 2 H_2 is directly represented as two copies of two conjoined circles), and there are multiple acceptable molecular representations that correspond to the same chemical equation. In contrast, the reverse translation requires recognizing that the balanced chemical equation is not a representation of the total number of particles of each species included in the image, which is what is explicit in the molecular representations, but rather the representation of a relationship of minimum proportions between reacting species and products formed in the reaction, which is implicit in such representations. The total number of particles of each species is an irrelevant feature for the translation that should be ignored. This example illustrates the role that the recognition, extraction, and use of relevant implicit information plays in reasoning about and with chemical representations with a mix of relevant/irrelevant and explicit/implicit features.

Similar reasoning challenges to the ones described above have been reported in studies focused on students' interpretation,

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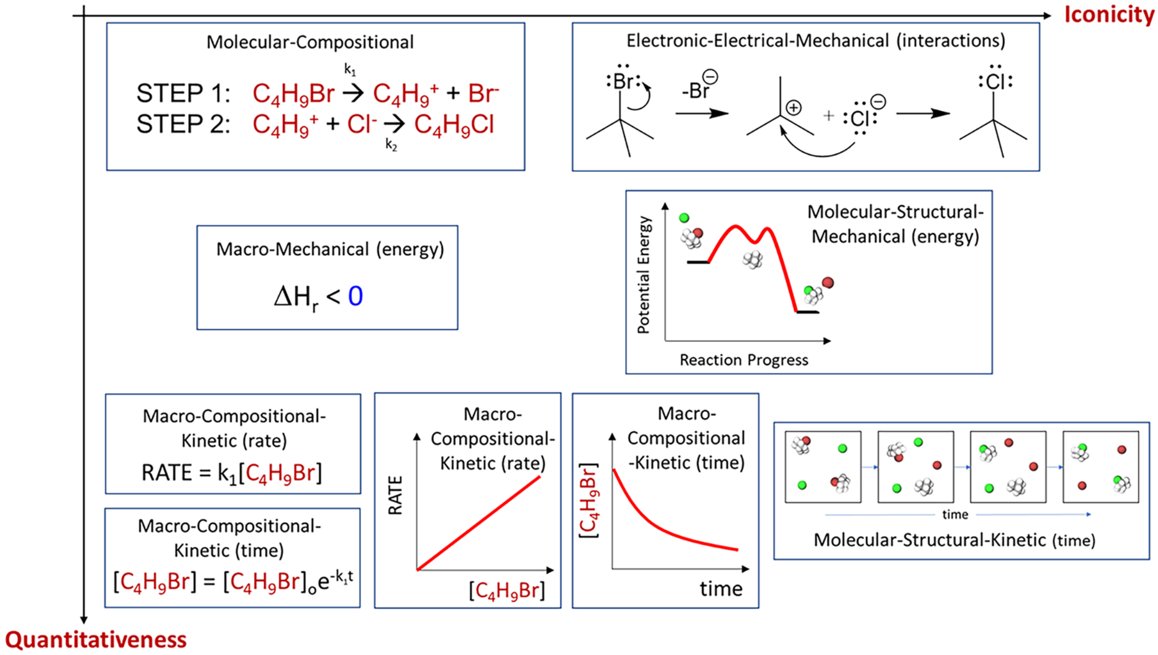

Figure 6. Chemical representations associated with the S_N1 reaction mechanism for a substitution reaction. The location and labeling of each representation seek to convey information about "distance" along the iconicity, quantitativeness, dimensionality, and granularity dimensions.

connection, generation, and use of more quantitative mathematical representations (e.g., translating from symbolic representations of mathematical functions to numerical tables to graph format and vice versa).[62,63,72,74,77,78] Mathematical formulas are more general, abstract, and dense in relevant features than graphical representations, which are more specific, concrete, and with a lower ratio of relevant to irrelevant attributes. Unpacking symbolic representations into graphic ones is more prone to procedural errors, such as substitution mistakes, while successfully packing graphical representations into symbolic ones is more sensitive to conceptual gaps or interpretation errors in the identification of relevant explicit (e.g., *y*-intercept) and implicit clues (e.g., slope of a line).[62,63]

Studies in math education suggest that reasoning challenges in connecting representations are also linked to the cognitive distance between those representations.[62,63] This is, the number of explicit or implicit steps associated with the translational act. For example, connecting the molecular formula of water to the molecular representation of intermolecular forces between water particles in Figure 4 is likely more cognitively demanding than connecting such a formula to the Lewis structure. More research is needed to determine how and to what extent cognitive demand in connecting representations may also be linked to distance within the iconicity, granularity, dimensionality, and quantitativeness dimensions. Some of these "distances" are made explicit in Figure 6, which illustrates various representations that can be built by unpacking the symbolic molecular-compositional representation of the S_N1 mechanism for a substitution reaction using periodic patterns (e.g., chlorine atoms are smaller and more electronegative than bromine atoms), procedural rules (e.g., mechanistic arrows are drawn from electron source to electron sink), and modeling primitives (e.g., shorter and more polar bonds are stronger, bond breaking is endothermic).

In Figure 6, distances along the iconicity and quantitativeness dimensions are represented by the relative position of each representation on the image, while distances along the other two dimensions must be inferred from the labels highlighting the corresponding granularity (macro → particulate → molecular → atomic → electronic) and dimensionality (compositional → structural → electrical → mechanical → kinetic) levels of each representation. One could expect that connecting representations farther from each other in this multidimensional space, as when translating the macro-compositional representation into the molecular-structural-kinetic representation, will be quite challenging for most of the students and will likely be mediated by the construction of other more proximate representations.[13] The farther the cognitive distance between representations, the higher the likelihood that multiple and diverse strategies, from imagistic to analytical, will need to be deployed to successfully complete the task.[79]

In general, the analysis presented in this section indicates that the unpacking and packing of chemical representations lead to changes not only in what is represented along the four major dimensions of iconicity, granularity, dimensionality, and quantitativeness but also in the:

- General (more abstract) versus more specific (more concrete) character of a representation.
- The ratio of relevant to irrelevant features that are represented.
- The number and types of features that are explicit or implicit in a representation.

All these factors can be expected to affect the interpretation, connection, generation, and use of chemical representations. The reasoning challenges that students are likely to face when engaged in any of these tasks could be conceptual, given the highly specialized knowledge needed to extract or infer the proper information in each situation, or procedural, given the need to identify and discriminate between relevant and irrelevant attributes and properly apply conventions and translational procedures. Challenges in connecting representations are likely to be exacerbated by the cognitive distance between representations. As described in the next section, an

https://doi.org/10.1021/jacsau.2c00498
JACS Au 2022, 2, 2658−2669

additional set of reasoning challenges is better characterized as cognitive-perceptual.

Cognitive-Perceptual Challenges in Reasoning about and with Chemical Representations

Research in cognitive psychology suggests that representational competency is built upon two interrelated competencies, namely, sense-making (or conceptual) competencies and perceptual competencies.[80] Sense-making competencies depend on knowledge and skills that help to connect or map visual features in a representation to relevant concepts to build inferences about the properties and behaviors of the entities or processes that are represented. In chemistry, sense-making processes rely on explicit conceptual and procedural knowledge of disciplinary conventions, known patterns, classification systems, procedural rules, chemical principles, and modeling primitives that support reasoning about and with chemical representations. The reasoning challenges described in the previous section are mostly related to sense-making processes.

Perceptual competencies, on the other hand, refer to the ability to quickly and effortlessly attach meaning to relevant visual cues in a representation.[80] These competencies demand fluency in both processing visual information included in a representation and connecting visual features across different types of representations. These types of competencies tend to develop inductively through exposure and experience working with many examples. They depend on reasoning that is often characterized as System 1 or Type I thinking in dual-process theories of judgment and decision-making.[81] This type of reasoning invokes processes that are automatic, fast, independent of working memory, and that are triggered and applied autonomously, without the need for controlled attention.

Type 1 reasoning relies on shortcut reasoning strategies, often called heuristics, that minimize cognitive load by facilitating the selection and reducing the number of cues considered in making a judgment or decision or by providing rules of thumb for how and where to look for relevant information.[82] These reasoning strategies may include intuitive heuristics, developed implicitly through personal interaction with the world, or expert heuristics developed through explicit and prolonged practice.[83] Intuitive heuristics are often effective cognitive tools that efficiently use information readily available to make choices or build inferences. They are responsible, however, for systematic errors in judgment (biases), particularly when relevant cues are implicit rather than explicit. Existing educational research in various STEM disciplines suggests that novice learners frequently activate intuitive heuristics when seeking to extract information and make sense of visual representations.[84−88] Experts in the discipline also rely on heuristic reasoning when engaged with representations, but they activate strategies systematized and internalized through disciplinary practice.

It is well-known that the intuitive heuristics that novices often use over-rely on the explicit features in a representation to build inferences about the properties or behaviors of represented objects or processes.[89] Explicit features are more salient to novices and thus more readily noticed. These features are particularly attention-grabbing when learners intuitively associate them to the properties or behaviors under analysis. For example, paying attention to the explicit total number of atoms in the chemical formulas of two different molecules will be quite appealing in building inferences about the relative boiling points of the associated substances to students who intuitively assume that larger and heavier molecules likely require higher temperatures to separate (or break apart). Explicit features also tend to be more easily and rapidly processed than implicit cues.[84,90] In the previous example, inferring the relative strength of intermolecular forces (IMFs) from chemical formulas can be expected to be a more cognitively taxing, and thus slower, task than simply counting the total number of atoms in the corresponding molecules.

Even if students consider both explicit and implicit features in their analysis of a representation, it is likely that their automatic inferences will be guided by the feature that is most salient and is processed the fastest. If this feature is relevant for completing the task, or if the inferences to which it leads are aligned with those derived from the analysis of relevant features, students may generate proper inferences (e.g., the larger molecules may also have the stronger IMFs and, thus, correspond to substances with higher boiling points). There are, however, plenty of reported examples in which heuristic reasoning based on explicit irrelevant features versus implicit relevant attributes in a representation lead to non-normative responses. This happens when, for example: paying attention to the explicit types and number of atoms represented in a molecular formula (compositional features) rather than to the implicit atomic connectivity and molecular geometry (structural features) to make inferences about emerging molecular properties (e.g., molecular polarity,[91] acid−base properties,[87] boiling and melting points,[85] nucleophilicity[68]); building inferences about the thermodynamic favorability of a reaction based on the explicit size and number of entities represented in a chemical equation rather than on the analysis of implicit changes in the types of chemical bonds and in the number of configurations that particles in the system can adopt;[86] or making judgements about the rate of change of a dependent variable y at point x in a graph based on its absolute value (explicit height on the graph) rather than on the value of its derivative at that point (implicit slope).[84]

Over-reliance on the analysis of salient and more easily processed explicit features is known to privilege heuristic judgments based on surface similarity between chemical representations.[85,88,92,93] Novice learners are thus likely to infer similar properties or behaviors for entities, systems, and processes whose representations share explicit features, ignoring or minimizing the effect of implicit features, such as the chemical nature of the species involved in a process, or less explicit features, such as the nature of the variables plotted in a graph. Intuitive heuristic reasoning is also often characterized by the tendency to reduce the number of features that are attended to and used to build interpretations.[94] In general, many chemistry learners tacitly reduce cognitive load by only recognizing or considering the effect of a single, most salient cue.[95] What is salient to a learner, however, will depend on the interplay between the specific features of a representation and a student's prior knowledge and experiences, which introduces variability in student reasoning within and across tasks. The salience of a feature will likely be influenced by intuitive assumptions about what properties of the represented entities determine the property or behavior under analysis (e.g., how the size of a molecule affects its stability[86]), by surface resemblance to known cases (e.g., interpreting a concentration vs time graph as a pH vs volume graph based on shape similarity[96]), particularly those cases that are somehow primed in a student's mind (e.g., recent exposure in classroom or lab), and by dominant recognition patterns in the human mind (e.g., vertical symmetry in objects is often more salient than horizontal symmetry[97]).

https://doi.org/10.1021/jacsau.2c00498
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The different examples presented in this section illustrate the central role that three interrelated associative processes, namely, associative activation, processing fluency, and attribute substitution, play in novices' reasoning about and with chemical representations.[98] Associative activation relies on connections between constructs in our minds to fill in information quickly and automatically based on judgements of resemblance to past observations or experiences. A construct may be retrieved first based solely on surface similarity to a current condition or due to its recent activation in a related situation. Processing fluency is determined by the subjective experience of effort required by a cognitive task.[90] Cues that are more salient and easier to process in a particular context are likely to grab an individual's attention and be assigned a greater weigh during reasoning. Attribute substitution triggers the automatic and unconscious evaluation of alternative attributes and may lead to the replacement of a less for a more readily accessible feature while building inferences or making judgments and decisions.

From this perspective, first interpretations of a chemical representation are likely to be triggered by its most salient and easily processed explicit features, such as the height or the width of the graph in an energy diagram.[84] These cues will activate related knowledge through associative activation. The more strongly activated constructs will likely be based on general intuitive correlations (e.g., more-A-more-B[99]) between salient attributes, although some of these attributes may be substituted for more readily accessible related variables. For example, when analyzing an energy diagram, the variable "reaction progress" may be interpreted as "time." As a result, when asked to infer which of two reactions is faster based on the analysis of their associated energy diagrams, some students may claim that reactions with a wider energy barrier will take more time to complete.[60] Attribution substitution seems to be quite common in the interpretation of some features in different types of chemical representations, including interpreting mechanistic arrows as connectors between molecules rather than representing movement of electrons,[100,101] associating arrows in atomic energy diagrams with electron translational motion rather than with electron spin,[24] or implicitly substituting speed for time when interpreting the *x*-axis in speed distribution graphs. This latter type of misattribution where the *x*-axis is interpreted as "time" in graphs displaying a dynamic feature of a system has been reported in diverse contexts.[19,60,84] It is important to recognize that heuristic reasoning may lead students astray even if they have the knowledge and ability required to generate the normative answers. In such cases, their interpretations may become more normative when prompted to reflect on and challenge their automatic response.[102]

Existing research suggests that experts also rely on heuristic reasoning to extract information and make sense of visual representations. The heuristics they use, however, are specialized strategies developed through prolonged practice and accumulation of domain knowledge. Repeated exposure to domain-relevant patterns allows them to quickly recognize and process complex chunks of information.[103] Rather than noticing and encoding individual explicit features of a representation, experts encode groups of components and their relationships as single "chunks" that automatically trigger conceptual schemas, procedural scripts, cognitive frames, or mental images that facilitate the interpretation, translation, generation, and use of a representation. For example, chemistry experts automatically detect the presence of functional groups in symbolic or iconic representations of molecules[95] and use them to make inferences about reactivity or light−matter interactions;[104] they tacitly recognize signal patterns in spectra and associate them with specific structural features in the molecules under analysis;[105,106] they implicitly detect symbolic forms in mathematical equations and link them to proper conceptual schemas[107] (e.g., detect the symbolic template [] = [] as indicative of equal amount or balancing influences); or they implicitly notice graphical forms in the shape of graphs that are quickly linked to relevant implicit information[17] (e.g., the steepness of a curve is associated with the rate of change of a represented dependent variable).

Perceptual fluency seems to strongly rely on visual chunking to sidestep typical visual working memory capacity and enhance performance by compressing information.[103] But the successful application of this strategy is highly constrained by domain knowledge. Experts are known to switch strategies when working with less familiar representations or types of tasks. With training, novice students may readily notice meaningful patterns in chemical representations but are likely to struggle to properly associate these noticed "chunks" to the domain knowledge that is most relevant in a particular context. For example, students may readily notice and highlight the presence of an OH group in a representation of methanol molecules (e.g., CH_3OH) but use this feature to infer that the substance may act as a strong base.[87] This suggests that perceptual fluency in the analysis of some representations may develop more rapidly than sense-making (conceptual) competency.

CONCLUSIONS AND IMPLICATIONS

The main goal of this Perspective was to provide a more in-depth analysis of distinctive characteristics of visual representations used in chemistry that can be expected to affect student reasoning about and with them. The four dimensions of variation in chemical representations identified in this work (iconicity, quantitativeness, dimensionality, granularity) point to different aspects of chemical representations that should be considered when thinking about how to best support students when learning to interpret, connect, generate, and use these visual tools to make sense of chemical systems and phenomena. Although using the chemistry triplet to frame the analysis and discussion of chemical representations has been quite productive in the chemistry education literature,[1,10,37] this approach does not always capture the complexity of reasoning that many instructional tasks demand from novice chemistry learners. It may also constrain the lenses used by chemistry education researchers in their analysis of data related to representational competency in our domain and the teaching strategies that instructors may use to foster it.

The ideas presented in this essay highlight the need for more careful consideration of the types of representational tasks in which students are asked to engage to properly scaffold their learning and to identify the specific reasoning challenges that they may face. Factors such as whether a task will demand the unpacking or packing of information (directionality of translation), the nature and number of explicit and implicit features that need to be analyzed, the density of relevant versus irrelevant elements to be considered, and the cognitive distance between representations to be connected along each of the four major dimensions of variation are likely to affect the cognitive demand of a task and interact in a significant manner with a learner's prior knowledge and experiences.

Domain knowledge and past experiences can be expected to have a major impact on learners' sense-making (conceptual) competencies[8] but also on their perceptual fluency.[80] One

https://doi.org/10.1021/jacsau.2c00498
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should not underestimate the critical role that intuitive heuristics play on novice students' reasoning about and with chemical representations, particularly when relevant inferential features in a representation are implicit, multiple elements need to be considered to build proper inferences, or the representation includes components that closely resemble those present in representations more familiar to the learner. These conditions may activate improper associations, reduce processing fluency, and foster attribute substitution that often leads students astray. Perceptual fluency increases when students learn to compress visual information into relevant chunks, but sense-making may be constrained by limited or weakly integrated domain knowledge.

The complexity of reasoning about and with chemical representations thus demands a more intentional and explicit approach to instruction in this area. Conventional teaching approaches in chemistry are frequently not guided by learning objectives that explicitly target representational competency. It is often tacitly assumed that students will learn to interpret, connect, generate, and use many chemical representations without explicit instruction that intentionally scaffolds the development of perceptual and sense-making competencies. Few instructors consciously reflect on specific teaching strategies that may best support the unpacking or the packing of visual information. Recent research studies point to the importance of designing instruction that explicitly targets both sense-making and perceptual fluency while paying careful attention to how individual differences in chemistry knowledge and experience may affect student reasoning.[30,31] Investigations in this area also highlight the need for a critical analysis of teacher-centered versus student-centered instructional strategies used to guide students in the unpacking/packing of chemical representations.[28,108]

Existing research in chemistry education has shown the positive effects that different types of tasks, such as compare-contrast[109] and drawing activities[13,25] as well as tasks that take advantage of adaptive technologies[110] or embodied cognition[111,112] (e.g., gestures, simulated action), have on different aspects of students' representational competency in chemistry. These investigations, however, typically do not consider how the distinctive characteristics and dimensions of different chemical representations interact with task characteristics to affect student performance. Given the rich and complex space spanned by the visual representations used in chemistry, more investigations are needed to characterize which instructional activities may be most effective in different contexts.

Similarly, more nuanced investigations could be carried out to better characterize how the different dimensions of variation and factors highlighted in this contribution affect student reasoning with chemical representations. Recent studies using eye-tracking techniques are providing insights into differences in leaners' perceptual fluency and factors that affect it.[84,104,113,114] Many of these investigations, however, do not differentiate participants' performance based on critical characteristics of the chemical representations under analysis. Existing studies related to students' sense-making competencies are varied but often guided by frames that are too broad and reduce the complexity of the targeted activities (e.g., characterizing a task as simply requiring a transformation between particulate and symbolic representations without paying attention to other dimensions). In general, more granular analyses would help us generate insights that more pointedly and effectively inform teaching practice in this area.

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Notes

The author declares no competing financial interest.

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