Capturing student reasoning about molecular structure and behavior

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UNIVERSITY OF MICHIGAN

What do we mean by reasoning?

What do we mean by reasoning?

Reasoning

noun

1. Thinking in which logical processes of an induction or deductive character are used to draw conclusions from facts or premises.

APA Dictionary of Psychology

What do we mean by reasoning?

Rank the following reactions from least favored to most favored:

1. $H_2S\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + HS^-\ (aq)$
2. $HCl\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + Cl^-\ (aq)$
3. $HI(aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + I^-\ (aq)$

The thinking process that occurs when we consciously try to solve a problem and/or logically draw conclusions about a phenomena.

Reasoning Studies in CER

- Reasoning using representations
- Mathematical reasoning
- Conceptual reasoning
- Mechanistic reasoning
- Chemical reasoning
- Argumentation

Anderson, T.R., et al. “Identifying and developing students’ ability to reason with concepts and representations in biology.” In Multiple representations in biological education. Springer, Doredrecht, 2013. 19-38

Moon, A. et al. “Analysis of inquiry materials to explain complexity of chemical reasoning in physical chemistry students’ argumentation” J. Res.Sci. Teach. (2017) 54 (10) 1322-1346

Rodriguez, J.; Towns, M. “Analysis of student reasoning about Michaelis-Mentin enzyme kinetics: Mixed conceptions of enzyme inhibition: Chem. Educ. Res. Pract. 2019, 20 (2) 428-442

K. Bain; Rodriquez, J.; Towns, M. Chemistry and Mathematics: Research and Frameworks to Explore Student Reasoning. J. Chem. Educ. (2019)

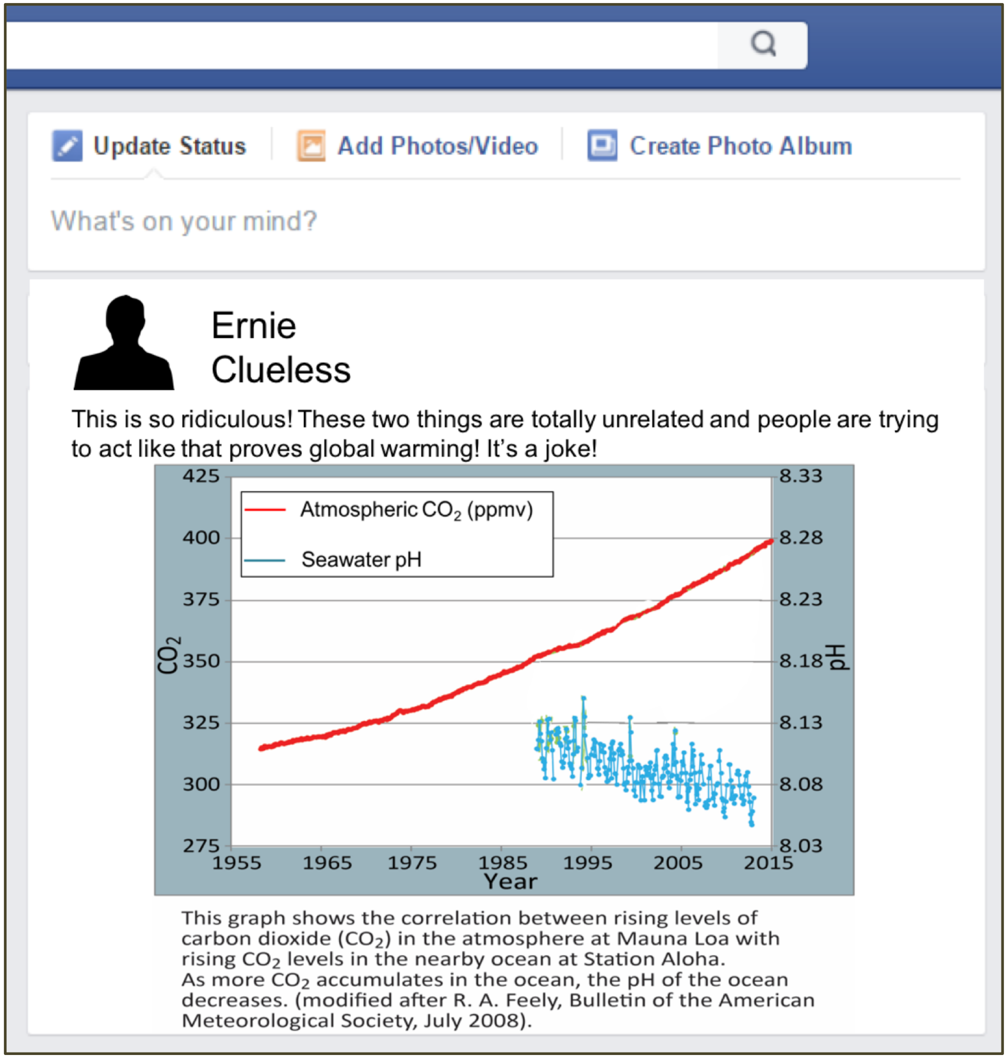
Kraft, Adam, Amanda M. Strickland, and Gautam Bhattacharyya. "Reasonable reasoning: multi-variate problem-solving in organic chemistry." *Chemistry Education Research and Practice* 11.4 (2010): 281-292.

Cooper M. M., Kouyoumdjian H., and Underwood S. M., (2016). Investigating Students’ Reasoning about Acid-Base Reactions *J. Chem. Educ.*, **93**(10), 1703–1712.

Capturing how students reason when they argue about climate change

Alena Moon

Writing about ocean acidification



Given the following equilibria:

$CO_2(atmos) \rightleftarrows CO_2\ (aq)$

$CO_2\ (aq) + H_2O\ (l) \rightleftarrows H_2CO_3\ (aq)$

$H_2CO_3\ (aq) \rightleftarrows H^+ + HCO_3^-\ (aq)$

$H^+ + HCO_3^-\ (aq) \rightleftarrows 2H^+ + CO_3^{2-}$

Explain the plot.

Argument Analysis

Cognitive Operations
Definition (1)
Observation (2)
Measurement (3)
Comparison (4)
Example (5)
Claim (6)
Consequences (7)
Cause and Effect (8)
Deduction (9)
Argumentation (10)

Increasing cognitive complexity

Single domain: Definition (1) – Comparison (4)

Two domains: Example (5) – Cause and Effect (8)

Multiple domains: Deduction (9) – Argumentation (10)

> Cognitive complexity increases with number of ontological domains and elements used and related

> Applied to 300 assignments

Grimberg, V.; Hand, B. Cognitive pathways: Analysis of students written texts for science understanding. Int. J. Sci. Educ. (2009) 31 (4) 503-521

Increasing cognitive complexity

Cognitive Operations
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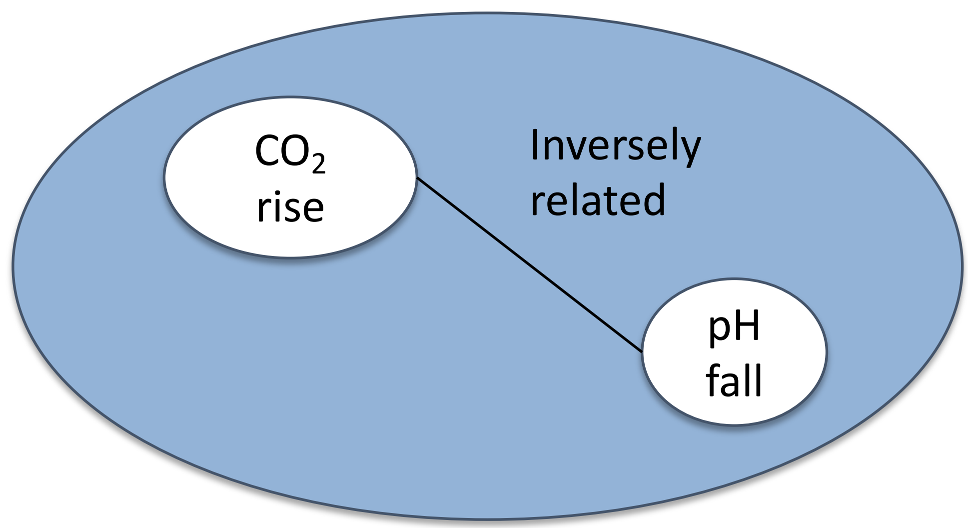
Comparison (4)
Example (5)
Claim (6)
Consequences (7)
Cause and Effect (8)
Deduction (9)
Argumentation (10)

Single domain

"The plot shown in your post shows that as the levels of atmospheric CO_2 rise, the pH of seawater falls, which means they are inversely related."



Increasing cognitive complexity

Cognitive Operations
Definition (1)
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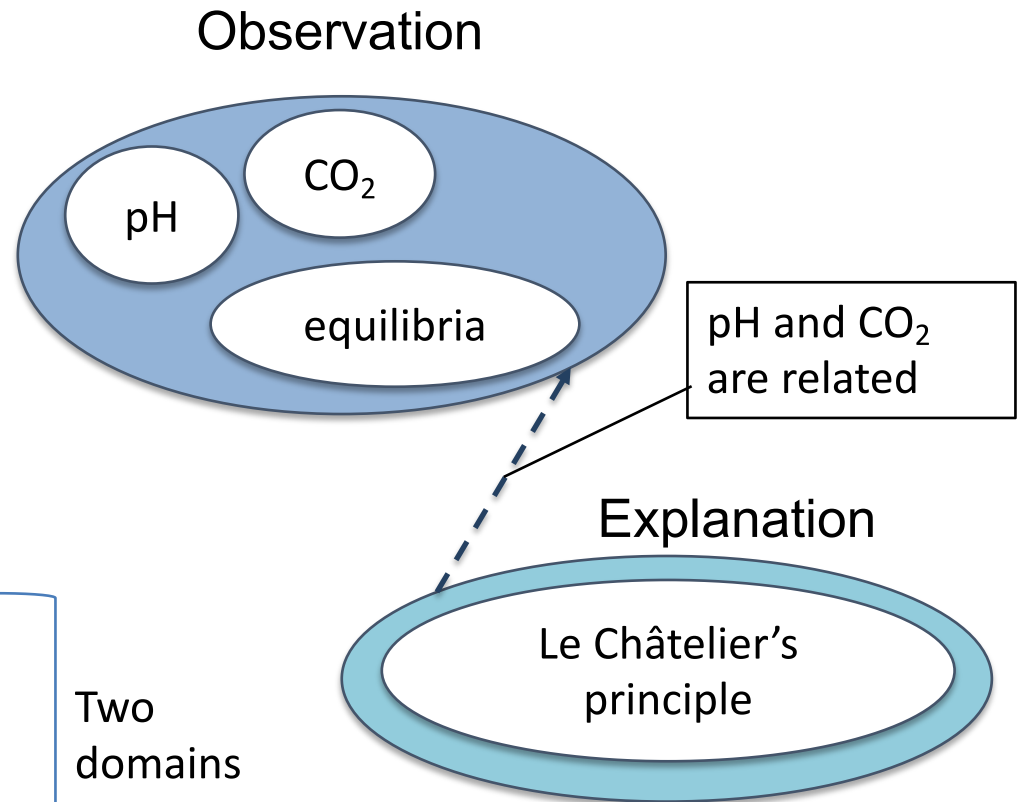
Two domains



"While it isn't known to all that pH and the concentration of CO_2 in the atmosphere is related, it actually is. Using the following set of equilibrium systems and Le Châtelier's Principle, this can be easily explained."

Relative frequency of operations

Operation	Frequency
Observation (2)	411
Claim (6)	348
Cause and effect (8)	331
Definition (1)	312
Comparison (4)	302
Deduction (9)	235
Consequences (7)	146
Argumentation (10)	63
Example (5)	51
Measurement (3)	34

Capturing Cognitive Complexity with a Single Metric

$$\text{Cognitive complexity} = \frac{\sum \text{(cognitive operation score * \# sentences used)}}{\text{total number of sentences}}$$

Relating cognitive complexity to other metrics

Variables	Cognitive Complexity
Number of operations	-0.649*
Final exam grade	-0.018
Final course grade	-0.025
CHEM placement	-0.081
MATH placement	-0.020
ACT math	0.003
GPA	-0.062
Gender	0.401
Ethnicity	0.071

* P (two-tailed) < 0.01

Note: students with higher cognitive complexity used fewer moves

There was no relationship between accuracy and cognitive complexity

complexity →

	Def.	Obs.	Meas.	Comp	Ex.	Claim	Cons.	C&E	Ded.	Arg.
# incorrect	9	11	0	13	1	8	6	40	18	4
# operations	312	411	34	302	51	348	146	331	235	63
% incorrect per total operations	3	3	0	4	2	2	4	10	8	6

Def. = definition
Obs. = observation
Meas. = measurement
Comp. = comparison
Ex. = example

Claim = claim
Cons. = consequences
C & E = cause and effect
Ded. = deduction
Arg. = argumentation

Comparison of Low vs. High Tier Assignments

- Using the average weighted complexity, assignments were divided into high, medium and low tiers

Low: 3.1 – 5.3
Medium: 5.4-7.6
High: 7.7-10

- Compared high and low tier assignments

Low complexity tier pattern

Cognitive operation	Paraphrase
Claim (6)	There is a simple reason atmospheric CO_2 levels and seawater acidity are related
Definition (1)	Le Chatelier's principle means when a system is in equilibrium it wants to stay there
Observation (2)	What is fighting the equilibrium is increased CO_2, changing the equilibrium levels of CO_2 in our atmosphere
Observation (2)	If there is more CO_2 in the atmosphere, there will be more contact with the water becoming aqueous CO_2. 71% of earth is covered by water
Observation (2)	With an excess of aqueous CO_2 in water the following reaction will be favored to occur: $CO_2(aq)+H_2O \rightarrow H_2CO_3$. Ocean water will be carbonized. That makes sense too; more CO_2 around water means there will be more carbonized water
Observation (2)	Carbonic acid dissociates in water to produce H^+ & $HCO_3^-(aq)$ and consequentially, this dissociates to H^+ & CO_3^{2-}
Cause and effect (8)	Therefore, carbonization of water produces hydrogen ions which float around in water, making water much more acidic, decreasing the sea's pH levels
Cause and effect (8)	As humans produce massive amounts of CO_2, CO_2 ends up in the oceans, in consequence, the oceans acidify.

High complexity tier pattern

Cognitive operation	Paraphrase
Deduction (9)	A change in the amount of carbon dioxide gas in the air is known to cause a shift in a thing called 'equilibrium'. The increase of carbon dioxide is going to cause a chemical reaction. This reaction will result in a shift in the increased concentration of carbon dioxide onto the other side of the equation in order to maintain a balance, or this 'equilibrium'. As more carbon dioxide gas is released into the atmosphere, the increased concentration in the air causes the gas to be dissolved into the ocean. The dissolved carbon dioxide gas then mixes with the water, causing a chemical reaction that results in the formation of carbonic acid, or H_2CO^3. The carbonic acid then loses its two hydrogen ions in two separate reactions, consequently creating the carbonate ion, $CO_3{}^{2-}$.
Cause & Effect (8)	The increase in hydrogen ions will decrease the water's pH
Definition (1)	The lower the pH is in a liquid, the more acidic the liquid is
Argumentation (10)	Therefore, we can conclude that the water is acidified due to the increase in atmospheric CO_2, and the graphic you posted is actually completely justified. According to your graph, the pH has dropped approximately 0.09 units. Although this is a small amount, think about how many tons of CO_2 emissions went into that change. Consider the fragility of the sea life and how even the smallest changes can destroy an entire ecosystem.

Patterns in low and high tier arguments

Low tier

Operation	No. of uses
observation	120
definition	107
comparison	94
claim	94
cause & effect	80
deduction	36
measurement	12
example	22
argumentation	2

High tier

Operation	No. of uses
claim	29
deduction	28
cause & effect	26
argumentation	22
definition	20
observation	18
consequences	17
comparison	14
example	4
measurement	1

Implications

- The adapted framework with complexity score provides a novel approach to holistically assessing student writing

- The framework can be applied to examine patterns in student writing
  - E.g. how likely is one operation to appear after another?

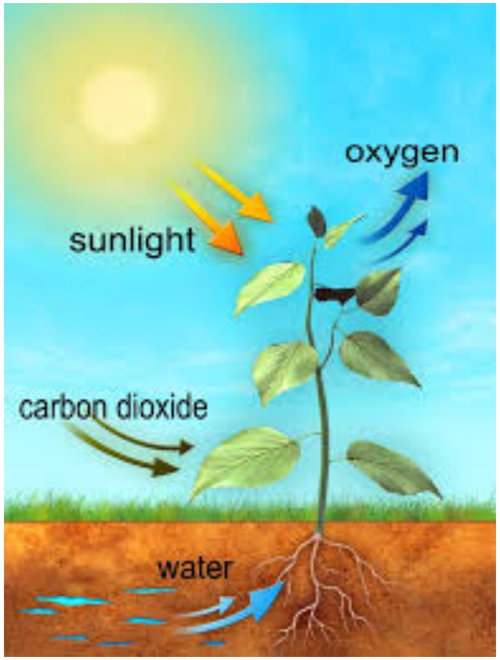
- The cognitive complexity metric appears to measure something unique
  - Students who perform well on typical performance measures don’t necessarily perform well on extensive writing tasks

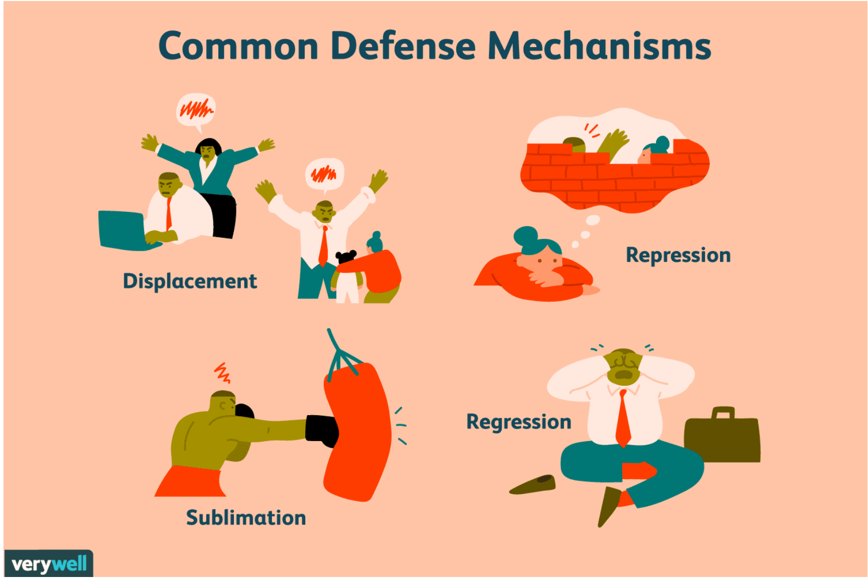
Moon, Alena, et al. "Application and testing of a framework for characterizing the quality of scientific reasoning in chemistry students' writing on ocean acidification." *Chemistry Education Research and Practice* (2019).

Capturing how students reason when they explain a reaction mechanism

Field Watts

Mechanistic Reasoning





- The primary work of scientists is to uncover the mechanisms underlying natural phenomena
- Mechanistic reasoning is 1) causal 2) built from experience; and 3) describes underlying structure

Russ R. S., Scherr R. E., Hammer D., and Mikeska J., (2008),. *Sci. Educ.*, **92**(3), 499–525

Mechanistic Reasoning

Mechanisms in organic chemistry

- Used to explain or predict outcomes of reactions

Requires process-oriented problem-solving

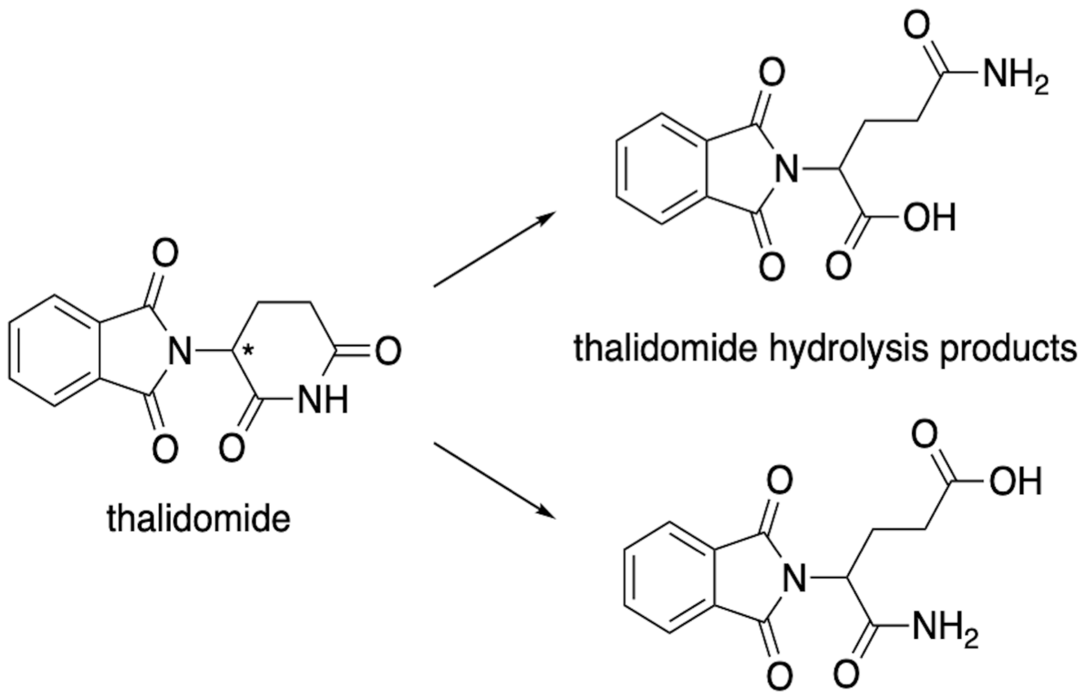
- Students are often more product-oriented in their problem-solving

There are many features students must consider when drawing a mechanism[3]

- Alternative reaction pathways
- The dynamic nature of chemical reactions
- Chemically reasonable steps

1. Bhattacharyya, G. *JCE*, **2013**, *90*(10), 1282-1289.
2. Graulich, N. *CERP*. **2015**, *16*, 9-21.
3. (a) Bhattacharyya, G.; Bodner, G.M. *JCE*. **2005**, *82*(9), 1402.; (b) Caspari, I.; Weinrich, M.L.; Sevian, H.; Graulich, N. *CERP*. **2018**, *19*, 42-59.; (c) Caspari, I.; Kranz, D.; Graulich, N. *CERP*. **2018**, *19*, 1117-1141.; (d) Popova, M.; Bretz, S.L. *JCE*. **2018**, *95*(7), 1806-1093.
4. Ferguson, R.; Bodner, G.M. *CERP*., **2008**, *9*, 102-113.

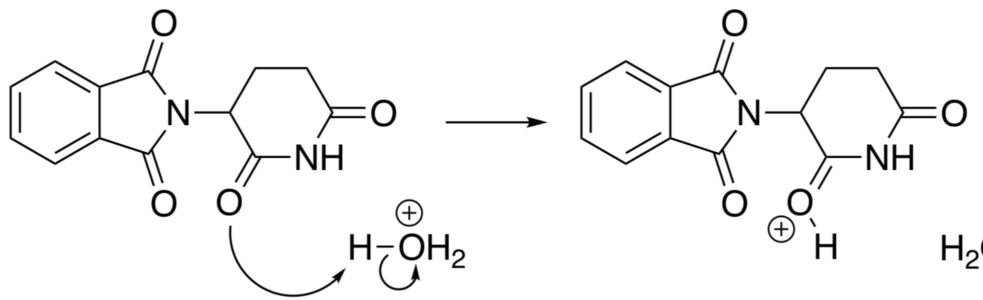
Developing a Therapeutic Analog for Thalidomide



500-754 word email proposal:

- Provided background about the drug **thalidomide**
- Identified **hydrolysis mechanism** that affects thalidomide
- Asked students to **describe the mechanism** to form both products
- Asked students to **propose an analog** that would prevent hydrolysis

Mechanistic Reasoning



Students are often **able to produce a correct mechanism** for common reactions, but there is evidence that they have **minimal understanding of the chemical reasoning** for particular steps.[2,4]

1. Bhattacharyya, G. *JCE*, **2013**, *90*(10), 1282-1289.
2. Graulich, N. *CERP*. **2015**, *16*, 9-21.
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Analytical Framework

Categories of Mechanistic Reasoning in Discourse

1. Describing the Target Phenomenon
2. Identifying Setup Conditions
3. Identifying Entities
4. Identifying Activities
5. Identifying Properties of Entities
6. Identifying Organization of Entities
7. Chaining: Backward and Forward

Russ R. S., Scherr R. E., Hammer D., and Mikeska J., (2008),. *Sci. Educ.*, **92**(3), 499–525.
Machamer, Peter, Lindley Darden, and Carl F. Craver. "Thinking about mechanisms." *Philosophy of science* 67.1 (2000): 1-25.
Caspari I., Kranz D., and Graulich N., (2018),. *Chem. Educ. Res. Pract.*, **19**(4), 1117–1141
Moreira P., Marzabal A., and Talanquer V., (2018), *Chem. Educ. Res. Pract.*, **20**(1), 120–131.

Analytical Framework

Categories	Code	Used at least once
Describing the target phenomenon	Overview of hydrolysis Identifies two reaction pathways	98 % 86 %
Identifying set up conditions	Specifies reaction medium Specifies carbonyls involved Static description of connectivity	74 % 55 % 82 %
Identifying activities	Describes electron movement Describes changes in bonding	99 % 100 %
Use of Chemistry Reasoning	Acid-base explanation Nucleophile-electrophile explanation Charge explanation Resonance explanation Electronegativity explanation	67 % 55 % 83 % 8 % 1 %

Units: single sentence

Russ R. S., Scherr R. E., Hammer D., and Mikeska J., (2008),. *Sci. Educ.*, **92**(3), 499–525.
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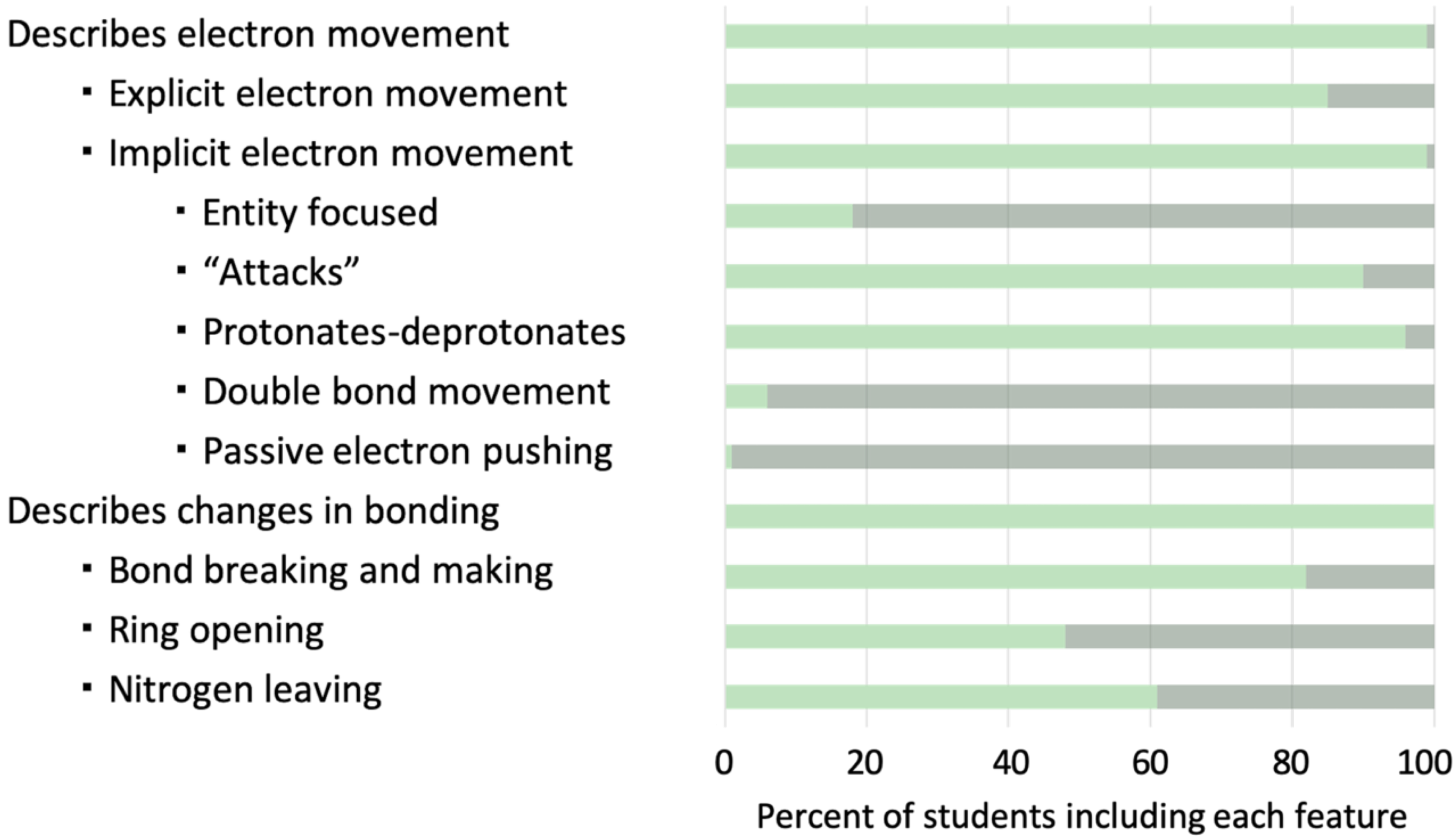
3 Identifying activities

included in **100%** of responses overall

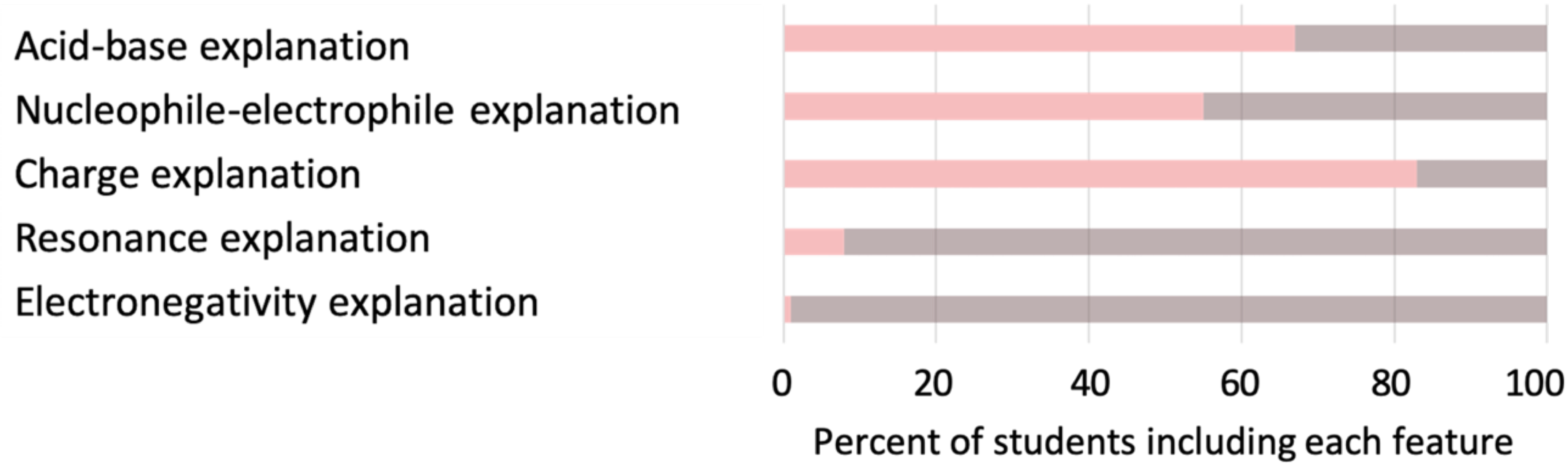


"The oxygen in the water molecule then attacks the carbon in the carbonyl, which, through electron pushing, forms a tetrahedral intermediate…"

4

Use of chemistry reasoning

included in **95%** of responses overall

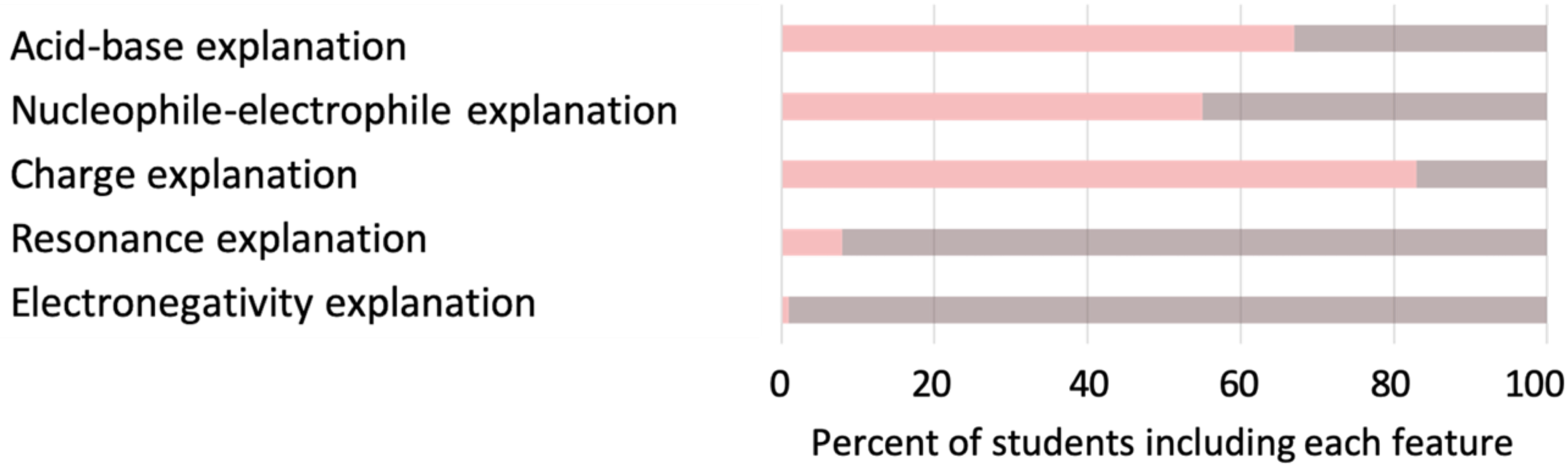


"Then, water, acting as a nucleophile, attacks the electrophilic carbon."

4

Use of chemistry reasoning

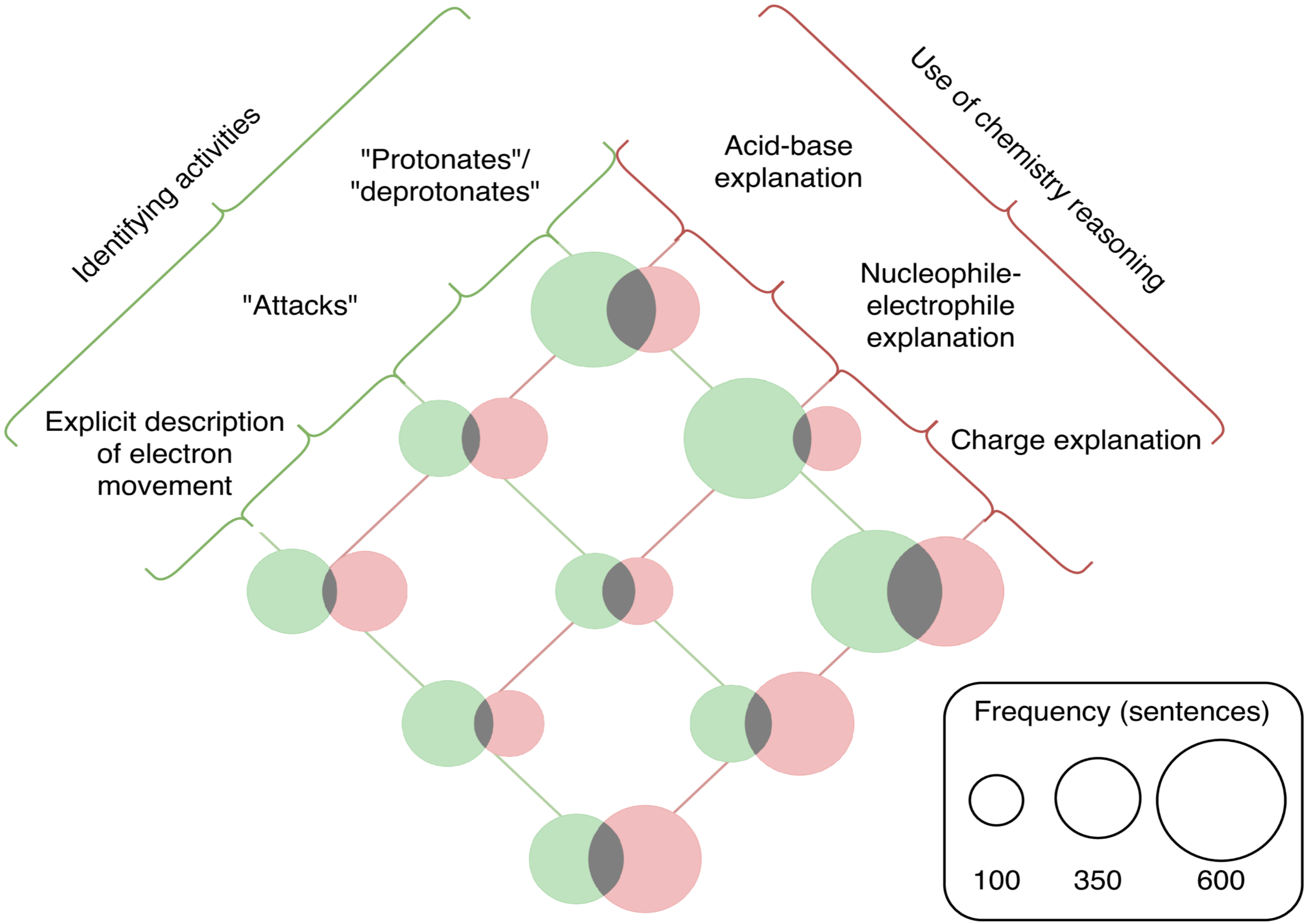
included in **95%** of responses overall



"Then, water, acting as a nucleophile, attacks the electrophilic carbon."

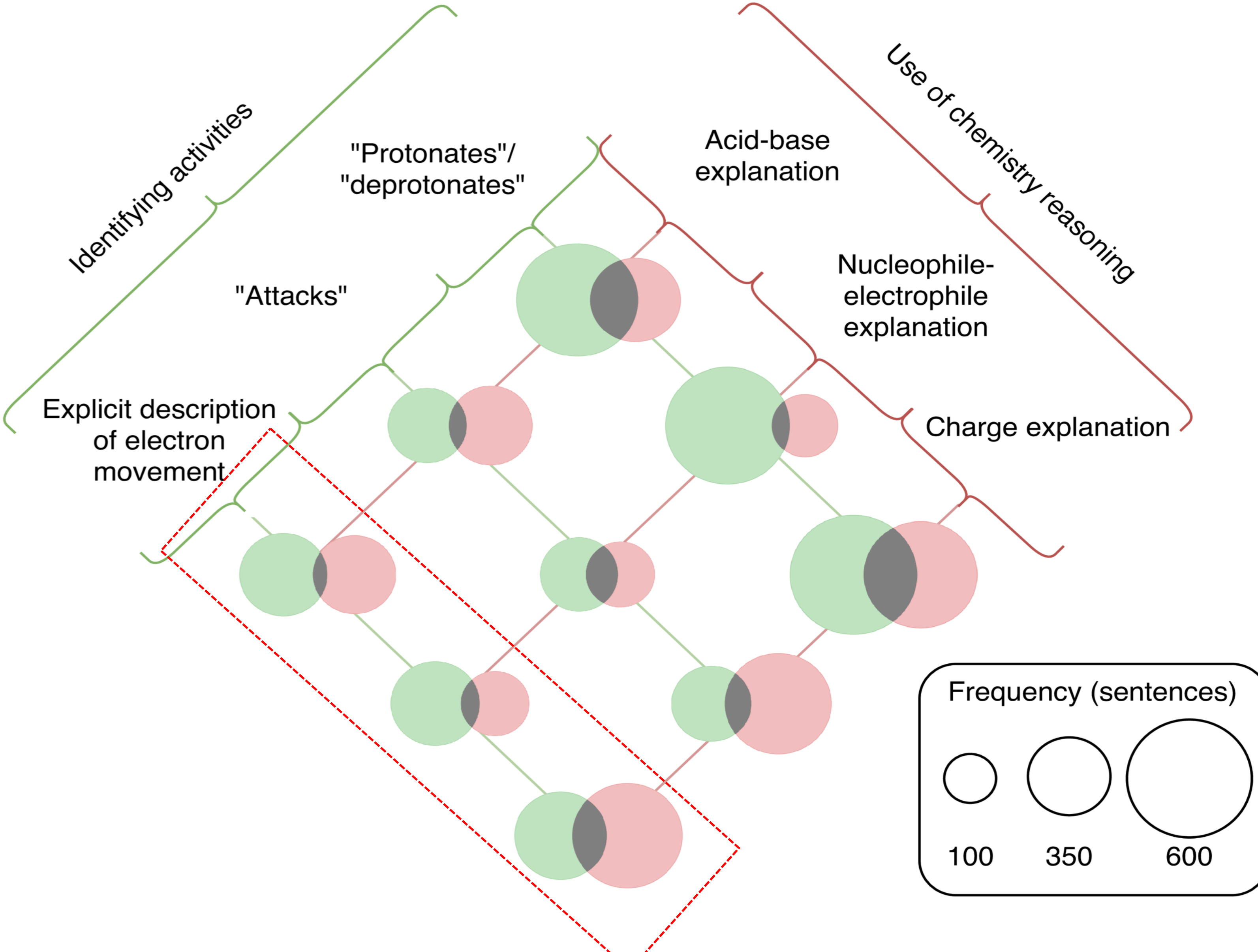
To what extent are students using mechanistic reasoning and chemical reasoning together?

Activities and Chemistry Reasoning



Overlap = number of sentence in which codes appear together

Activities and Chemistry Reasoning



Overlap = number of sentence in which codes appear together

Capturing Co-occurrence

"Lift": an association rule which measures the degree of dependence between two items

$$\text{Lift} = \frac{P(A,B)}{P(A) \cdot P(B)}$$

Where
P(A,B) = probability of code A and code B appearing together
P(A) = probability of code A appearing
P(B) probability of code B appearing

Lift < 1: codes appear together less often than expected

Lift > 1 : codes appear together more often than expected

i.e. Lift = 2 means the codes appear together twice as often as expected due to chance

Dillon, John, et al. "Student Emotion, Co-Occurrence, and Dropout in a MOOC Context." *International Educational Data Mining Society* (2016).

Case: Co-occurrence of explicit electron movement and chemical reasoning

Chemical Reasoning Code	Lift
Acid-base explanation	0.51
Nucleophile-electrophile explanation	4.14
Charge explanation	1.49

Students were less likely relate electron movement to acid-base explanations for the Thalidomide hydrolysis mechanism

Lift < 1: codes appear together less often than expected

Lift > 1 : codes appear together more often than expected

Case: Co-occurrence of explicit electron movement and chemical reasoning

The carbonyl group between the two nitrogens lowers the acidity of the molecule (electron density being able to move toward the oxygen makes it more reactive) so it can be protonated (adds hydrogen, H) by hydronium (H3O+) which creates a positive oxygen. Next, water will deprotonate (molecule loses hydrogen) the stereocenter so that carbon-carbon double bond is formed within the six membered ring between the carbon that use to be stereocenter and the carbonyl oxygen (the oxygen will become neutral and is now part of an alcohol group, OH). After a water will deprotonate the alcohol group so the double bond of the oxygen reforms and a hydronium will protonate the stereocenter to create the S-stereocenter.

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- Students are appealing to Bronsted-Lowry model more than Lewis model
- Their discussion of electron movement tends to be implicit rather than explicit when using Bronsted-Lowry

Implications

- The adapted framework with Lift metric provides a way to explore how students are using chemistry ideas in their reasoning about mechanisms

- The framework and metric can be applied to examine patterns in student writing
  - E.g. how likely are students to explicitly describe electron movement when appealing to the Bronsted-Lowry model?

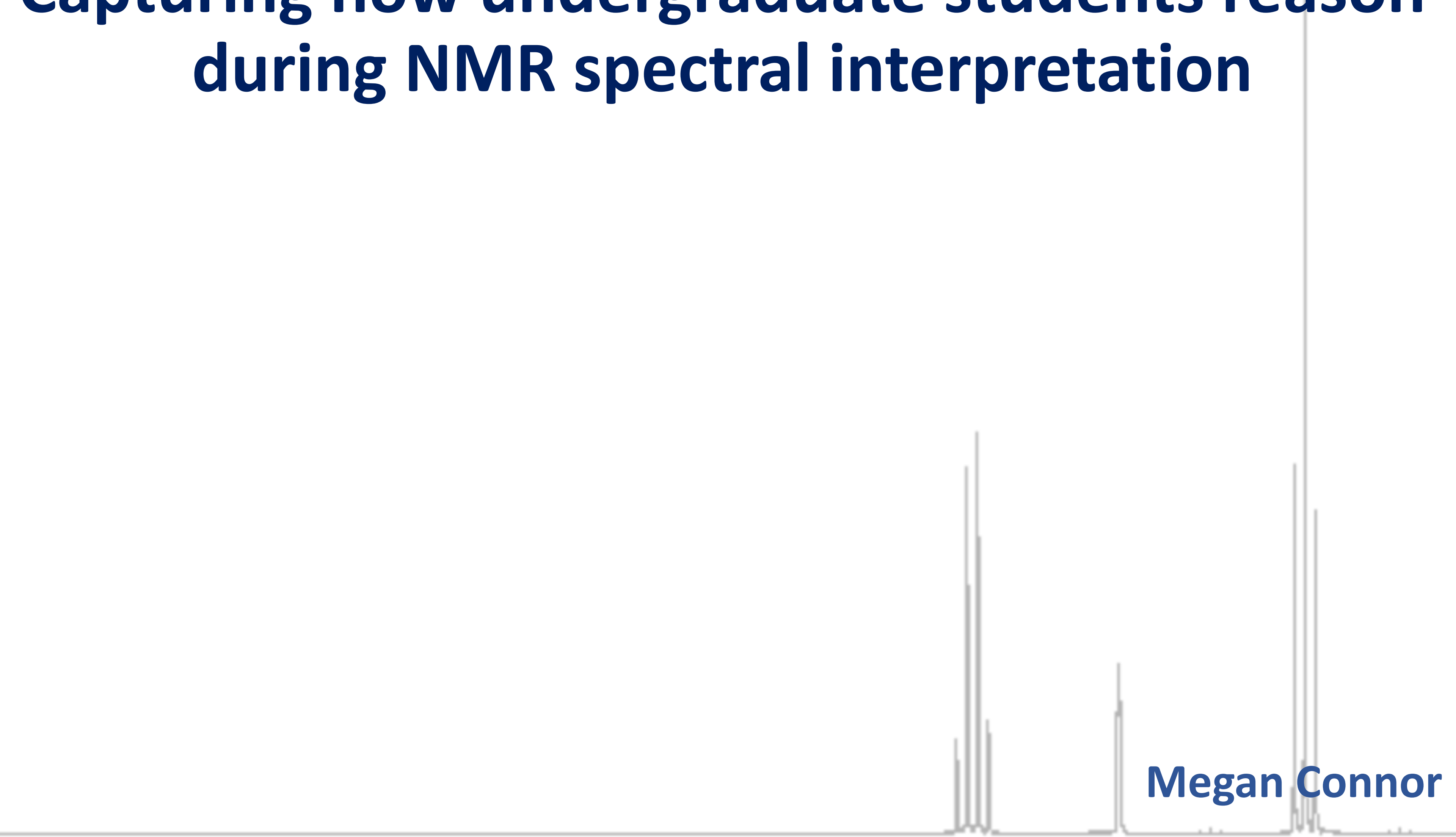
Watts, F. et al “What students write about when students write about mechanisms: Analysis of features present in students’ written descriptions of an organic reaction mechanism” Chem. Educ. Res. Pract., submitted

Lingering Questions

- How do these frameworks and metrics function when student are engaging with other types of arguments or reasoning about other types of chemical phenomena?

- What features of assignment prompts elicit more complex arguments or mechanistic reasoning about chemical phenomena?

Capturing how undergraduate students reason during NMR spectral interpretation



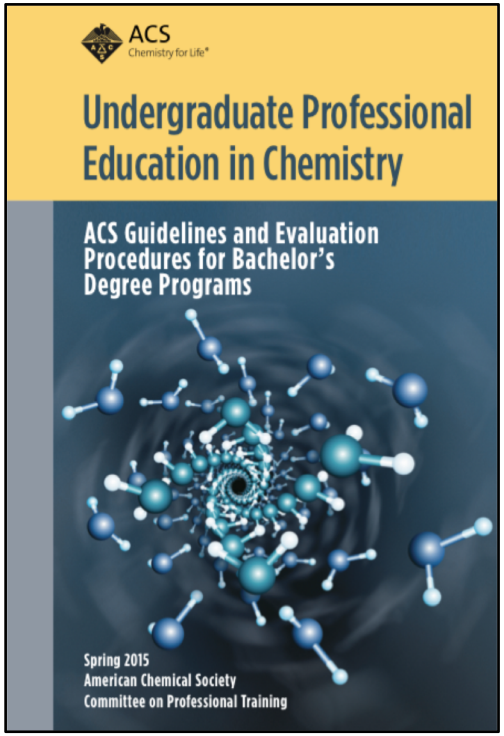
Megan Connor

NMR Spectroscopy in the Chemistry Curriculum

- Essential technique to elucidate the structure of molecules
- Difficult to teach and learn; requires understanding of multiple concepts and complex problem solving skills
- We need to know more about how students learn to interpret spectra and how instructor's learn to teach this topic

ACS Guidelines (2015) American Chemical Society; Washington D.C.
Cartrette, D. P., and Bodner, G. M. (2010), Non-Mathematical Problem Solving in Organic Chemistry, *J. Res. Sci. Teach.*, 47, 643–660

NMR Spectroscopy in the Chemistry Curriculum

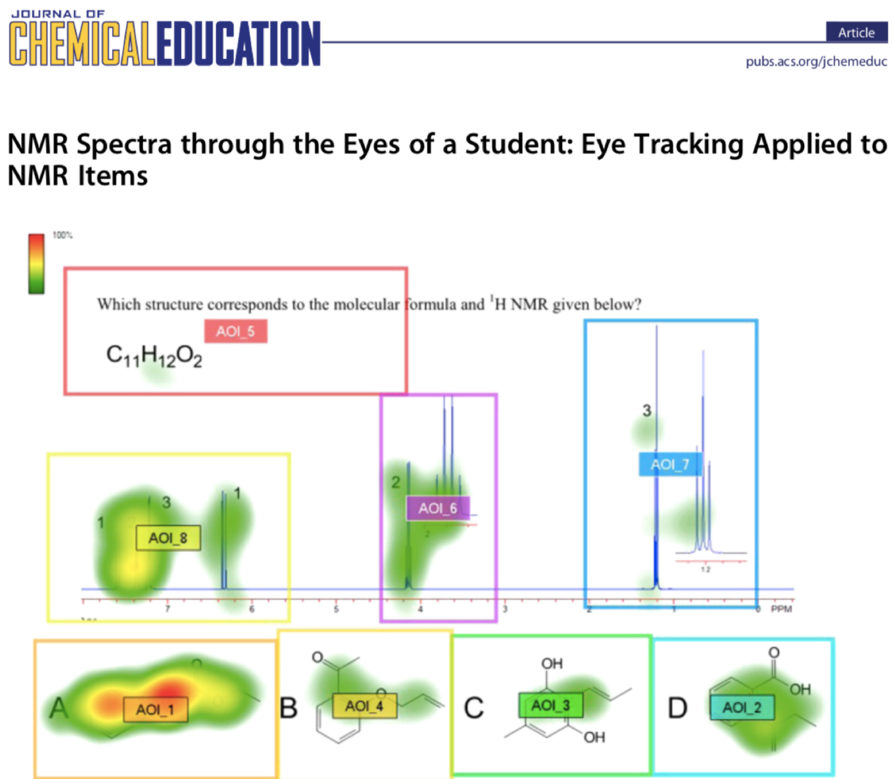


"Approved programs *must* have a functioning NMR spectrometer on site that undergraduates use….If the on-site instrument does not meet all of the program's research needs, stable arrangements must be made with proximal sites to provide ready access to appropriate NMR instrumentation[1]."

American Chemical Society, (2015), *Undergraduate professional education in chemistry: ACS guidelines and evaluation procedures for bachelor's degree programs*
Simpson et al., 2015, *J. Chem. Ed.* , 92, 693-697.
Topcszewski et al., 2017, *J. Chem. Ed., 94, 29-37.*

NMR Spectroscopy in the Chemistry Curriculum

- The majority of publications report teaching ideas
- Only a few studies examining how this complex topic is learned



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NMR spectral interpretation as "non-mathematical problem solving"

JOURNAL OF RESEARCH IN SCIENCE TEACHING VOL. 47, NO. 6, PP. 643–660 (2010)

Non-Mathematical Problem Solving in Organic Chemistry

David P. Cartrette, George M. Bodner

Department of Chemistry, Purdue University, West Lafayette, Indiana 47907

More successful participants were more likely to:

- Use consistent approaches
- Draw fragments as they worked
- More carefully mine spectral data
- Check their final answer

NMR spectral interpretation when arguing from evidence

JOURNAL OF CHEMICAL EDUCATION
Article
Cite This: *J. Chem. Educ.* 2019, 96, 2072–2085
pubs.acs.org/jchemeduc

Arguing from Spectroscopic Evidence

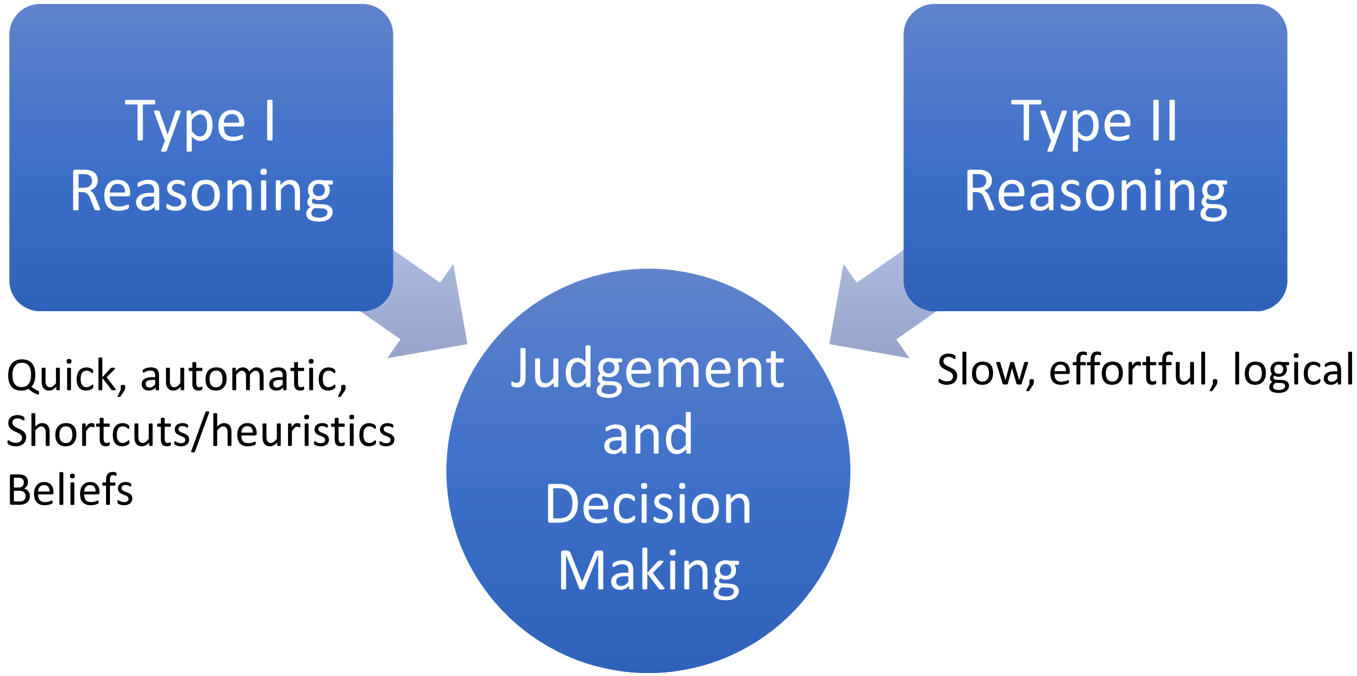
Ryan L. Stowe*,† and Melanie M. Cooper

Department of Chemistry, Michigan State University, 578 South Shaw Lane, East Lansing, Michigan 48824, United States

Analyzed responses to assessment items:

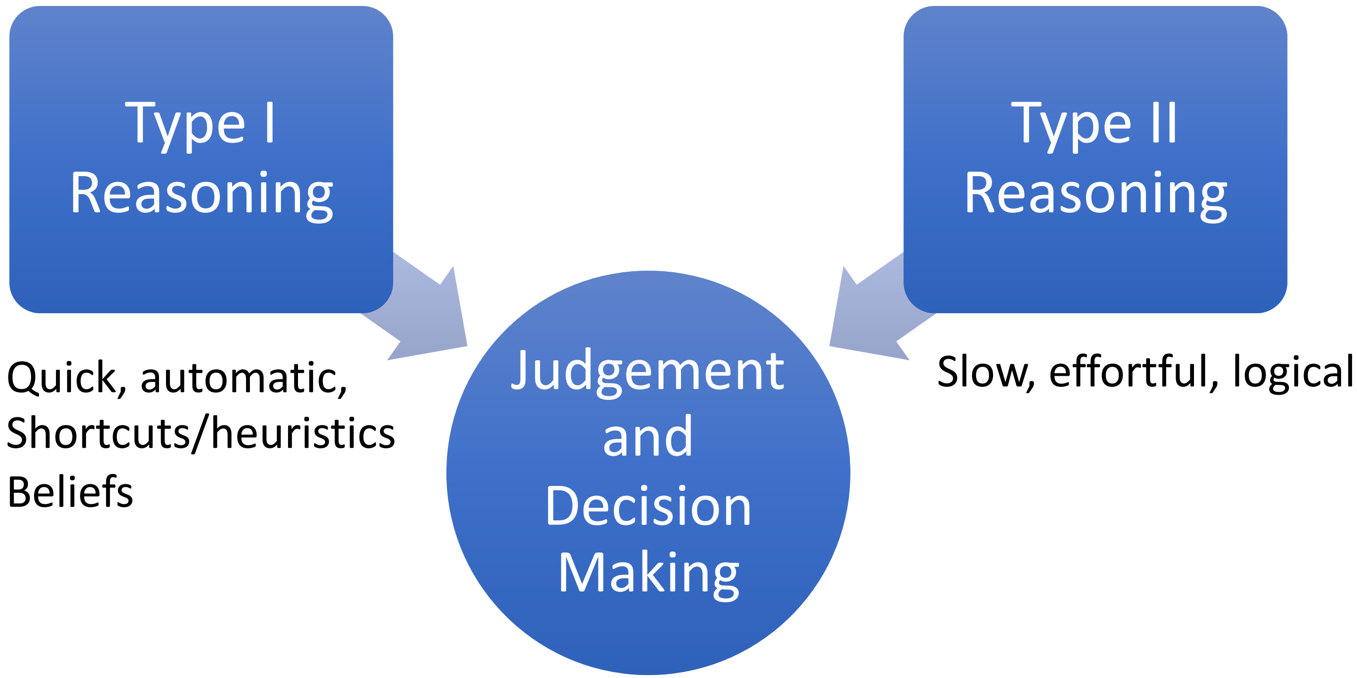
1. Students could analyze and interpret data from Infrared, ^{13}C NMR, and ^{1}H NMR traces when prompted to pull specific information
2. Students success in completing these tasks was not associated with their success in constructing evidence based claims
3. Assessment prompt structures had no impact on student success in constructing evidence based claims

Dual Process Theory



Maeyer and Talanquer, 2013, *J. Res. Sci. Teach.*, 50, 748-767.

Dual Process Theory

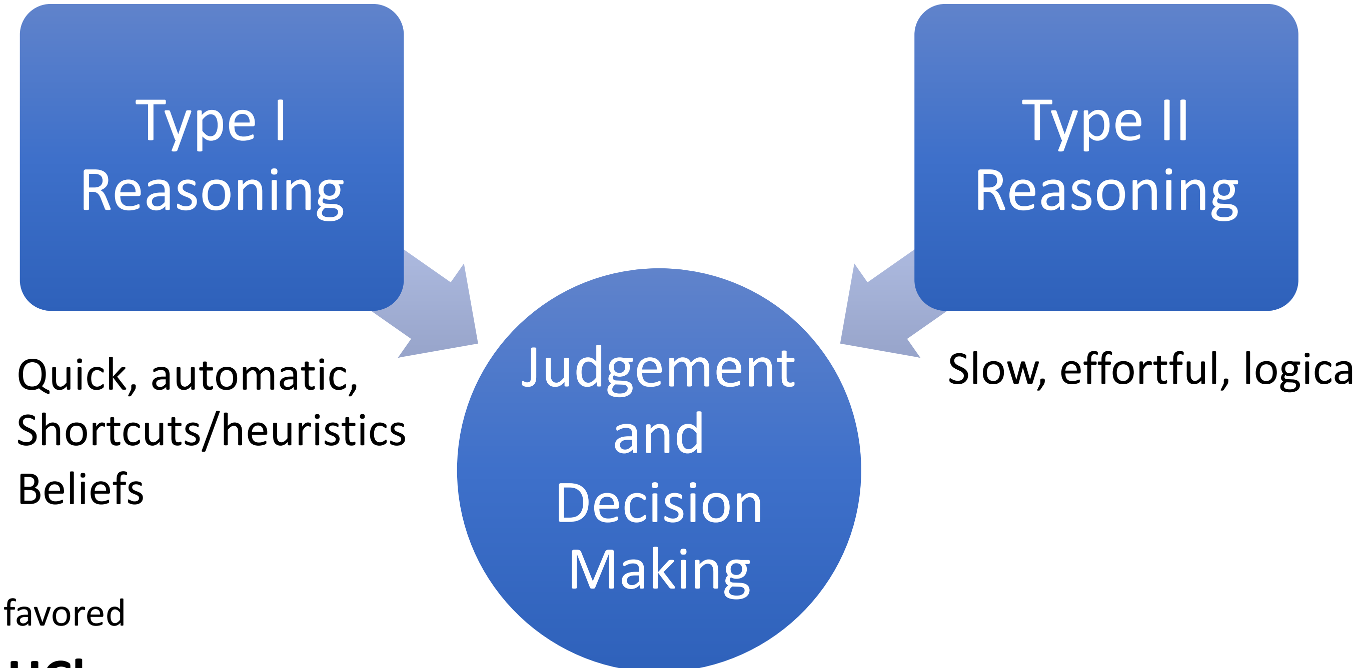


Rank the following reactions from least favored to most favored:

1. $H_2S\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + HS^-\ (aq)$
2. $HCl\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + Cl^-\ (aq)$
3. $HI(aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + I^-\ (aq)$

Maeyer and Talanquer, 2013, *J. Res. Sci. Teach.*, 50, 748-767.

Dual Process Theory



Least to most favored

H_2S, HI, **HCl**

Rank the following reactions from least favored to most favored:

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2. $HCl\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + Cl^-\ (aq)$
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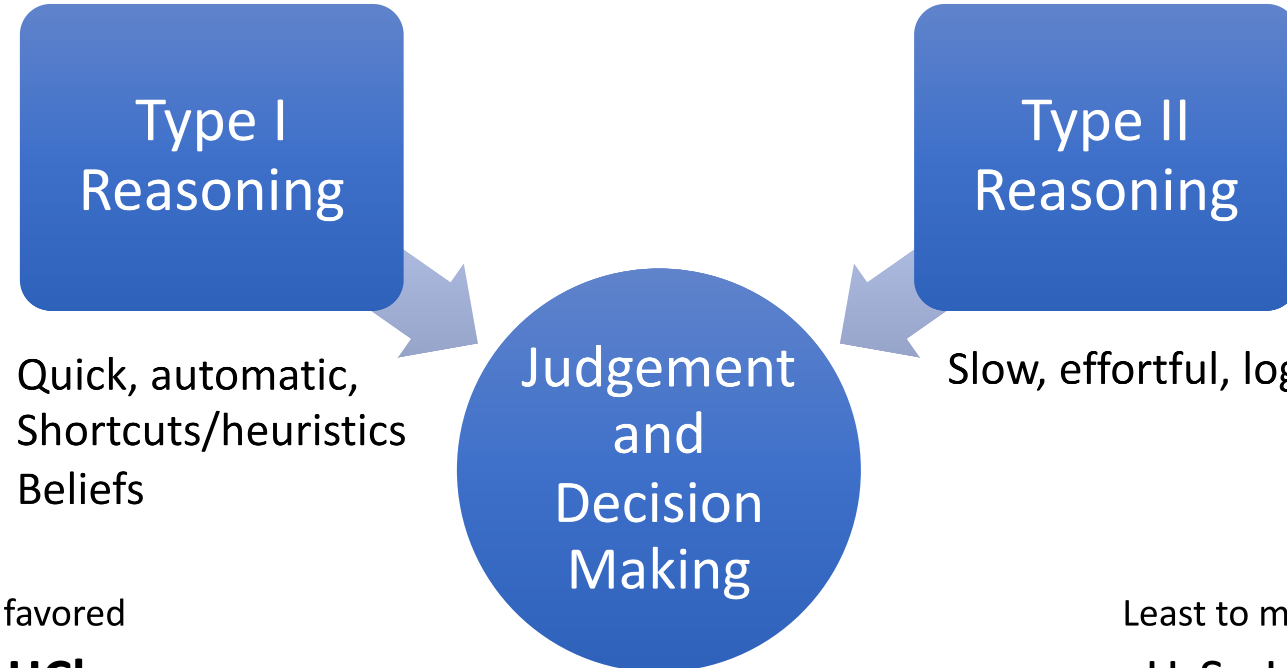
Maeyer and Talanquer, 2013, *J. Res. Sci. Teach.*, 50, 748-767.

Dual Process Theory



Quick, automatic,
Shortcuts/heuristics
Beliefs

Slow, effortful, logical

Least to most favored

H_2S, HI, **HCl**

Least to most favored

H_2S, HCl, **HI**

Rank the following reactions from least favored to most favored:

1. $H_2S\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + HS^-\ (aq)$
2. $HCl\ (aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + Cl^-\ (aq)$
3. $HI(aq) + H_2O\ (l) \rightleftarrows H_3O^+\ (aq) + I^-\ (aq)$

Maeyer and Talanquer, 2013, *J. Res. Sci. Teach.*, 50, 748-767.

Conceptual Understanding and Modes of Reasoning

Students' understanding of NMR principles

Sophisticated reasoning

- Identifies and assesses all relevant spectral cues
- Relies on valid chemical assumptions

Conceptual Understanding

1. Valid chemical assumptions
2. Invalid chemical assumptions (problematic Type 2 reasoning)*

Modes of Reasoning

1. Productive reasoning strategies
2. Unproductive reasoning strategies (problematic Type 1 reasoning)*

Maeyer and Talanquer, 2013, *J. Res. Sci. Teach.*, 50, 748-767

Data Collection

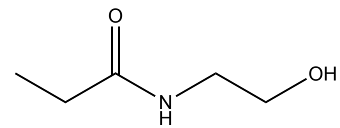
Developed spectral interpretation tasks that incorporate difficult features and authenticity for undergraduates

1. Difficult features identified through faculty interviews

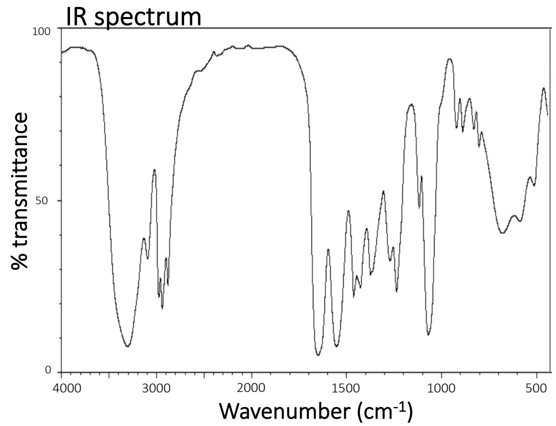
2. Developed three tasks using literature on day-to-day problems of practicing chemists[6]

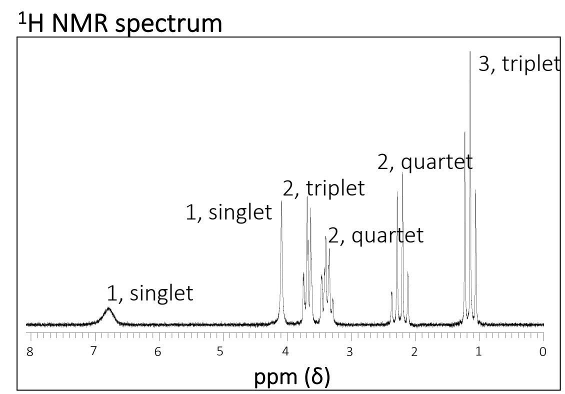
3. Piloted to ensure a range of difficulty

Chemists conducted a series of reactions to synthesize N-(2-hydroxyethyl)-propanamide. The chemists then analyzed the final product spectroscopically to determine if the synthesis was successful. Based on the spectroscopic data of the final product below (IR and ^{1}H NMR spectra), did the chemists successfully synthesize N-(2-hydroxyethyl)-propanamide?



N-(2-hydroxyethyl)-Propanamide





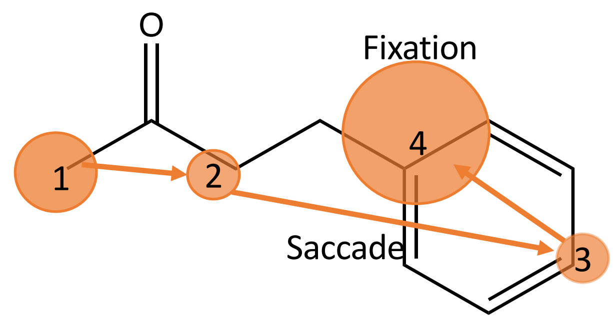
Raker and Towns, 2012, *Chem. Educ. Res. Pract.*, 13, 179-185.

Data Collection

Eye tracking and retrospective think-aloud interviewing with 18 undergraduate students

Participants and setting

- 18 undergraduates
- Organic Chemistry II Laboratory



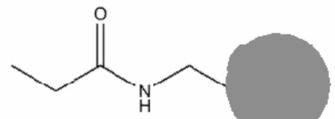
Eye tracking and retrospective think-aloud interviewing

- Common tools for investigating cognitive processing strategies
- Eye tracking provides insight into visual attention and viewing patterns
- Retrospective think-aloud interviewing provides insight into reasoning

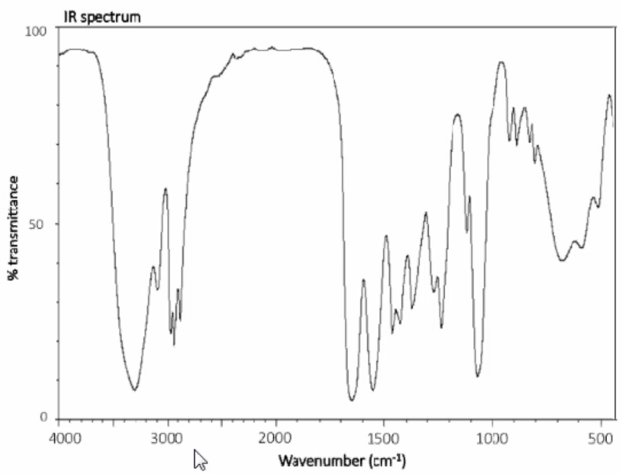
Tobii Pro X3-120 screen-based eye tracker
Sampling frequency: 120 Hz
Minimum fixation duration: 100 ms

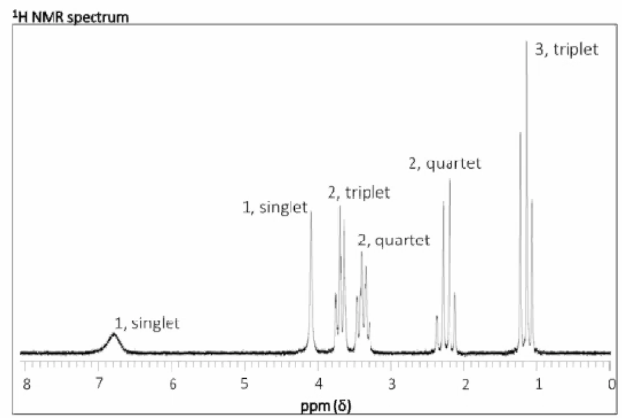
Data Collection

Chemists conducted a series of reactions to synthesize N-(2-hydroxyethyl)-propanamide. The chemists then analyzed the final product spectroscopically to determine if the synthesis was successful. Based on the spectroscopic data of the final product below (IR and ^{1}H NMR spectra), did the chemists successfully synthesize N-(2-hydroxyethyl)-propanamide?



N-(2-hydroxyethyl)-Propana





Data Analysis: Analyzed Retrospective Think-aloud interviews for Cognitive Constraints

Two researchers coded all responses for **assumptions** and **common heuristics**

↓

Codes were discussed and refined until 100% agreement reached

↓

Identified themes among assumption codes

↓

Consulted external experts for validity

Talanquer, 2014, *J. Chem. Ed.*, 91, 1091-1097.

Results: Retrospective Think-aloud Interviews

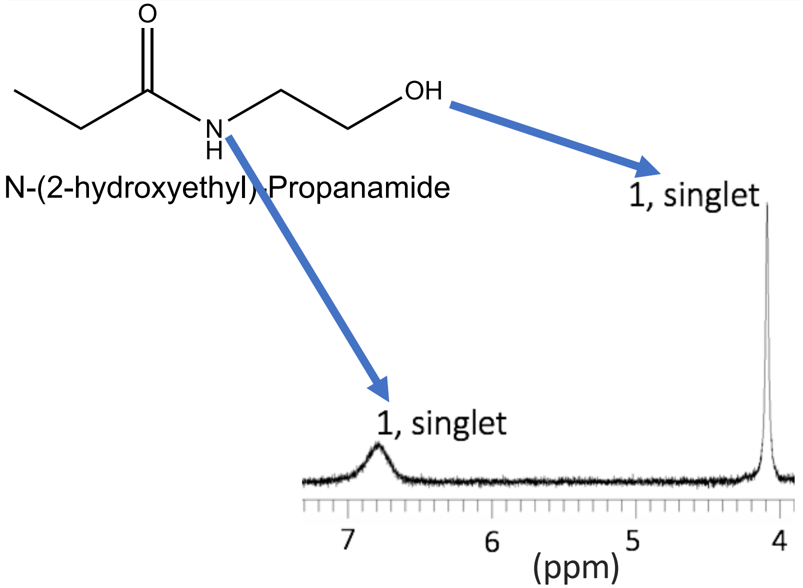
Invalid chemical assumptions

Number of participants (n) contributing to theme

Theme	n
Assumptions that the "N+1 rule" should hold	13
Assumptions that spectral data should be absolute	9
Practical invalid assumptions	8
Visuospatial invalid assumptions	7
Fundamental invalid assumptions	6

$N_{Total} = 18$

Assumptions that the "N+1" rule should hold



Invalid chemical assumption: NH and/or OH should not appear as singlets

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Results: Retrospective Think-aloud Interviews

Invalid chemical assumptions

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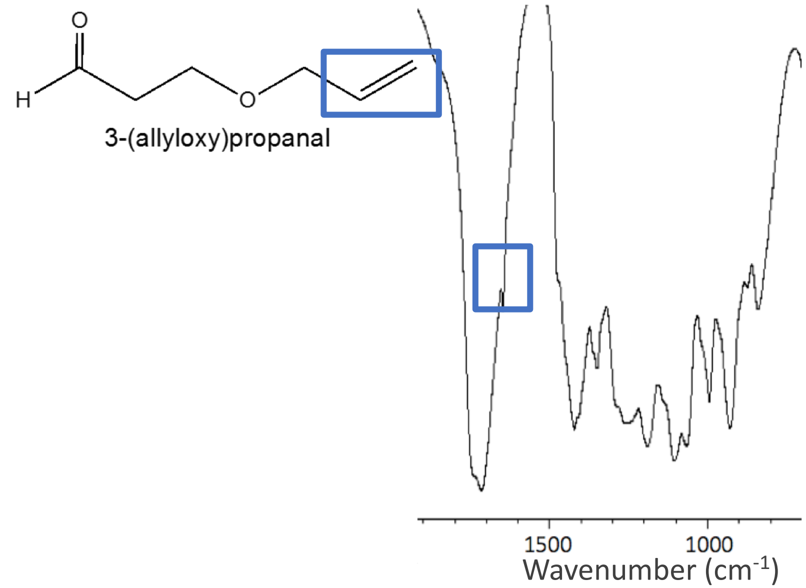
Fundamental invalid assumptions	6

$N_{Total} = 18$

Assumptions that spectral data should be absolute



Invalid chemical assumption: IR peaks should be prominent if the functional group is present

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Results: Retrospective Think-aloud Interviews

Invalid chemical assumptions

Number of participants (n) contributing to theme

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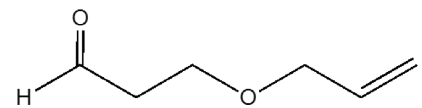
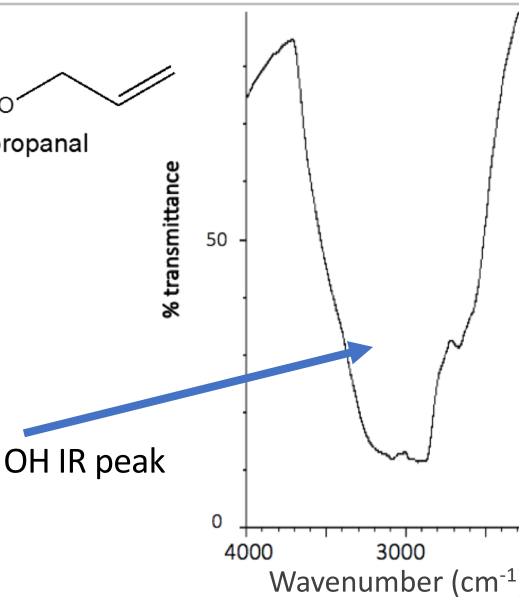
Fundamental invalid assumptions	6

$N_{Total} = 18$

Practical invalid assumptions



3-(allyloxy)propanal



Invalid chemical assumption: The large IR peak near 3000 cm^{-1} corresponds to the CH functional group

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Results: Retrospective Think-aloud Interviews

Invalid chemical assumptions

Number of participants (n) contributing to theme

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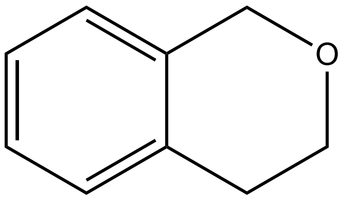
Fundamental invalid assumptions	6

$N_{Total} = 18$

Visuospatial invalid assumptions



isochroman

"And, then I moved straight to NMR. See what I did. Here's what I counted, right off the bat, the peaks. The phenyl I counted wrong a bunch of times because of the symmetrics. There should be two on the phenyl. Three on the other ring. Three. That lined up good with that." – Participant 17

Invalid chemical assumption: Isochroman possesses molecular symmetry

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Results: Retrospective Think-aloud Interviews

Invalid chemical assumptions

Number of participants (n) contributing to theme

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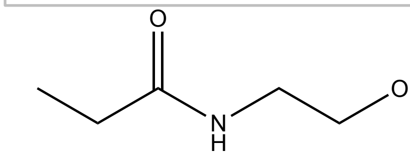
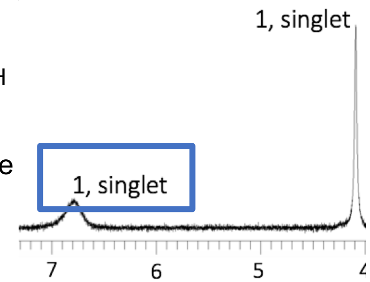
Visuospatial invalid assumptions	7
Fundamental invalid assumptions	6

N_{Total} = 18

Fundamental invalid assumptions



N-(2-hydroxyethyl)-Propanamide



"And since that NH singlet in the NMR is not very strong, my thought process was that it's possibly just a really low concentration of that molecule that might be present. But I wasn't really sure what else could be there if it was a low concentration of just that specific molecule." – Participant 4

Invalid chemical assumption: Specific parts of a molecule may vary in concentration

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Results: Retrospective Think-aloud Interviews

Heuristic reasoning strategies

One-reason decision making:

"And then, I basically, I concluded that… those peaks couldn't be singlets. My reasoning for the question."

Common heuristics[7]

1. One-reason decision making
2. Rigidity
3. Generalization
4. Processing fluency
5. Associative activation
6. Affect
7. Representiveness
8. Reduction
9. Overconfidence
10. More A – More B

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Talanquer, 2014, *J. Chem. Ed*.

Results: Retrospective Think-aloud Interviews

Heuristic reasoning strategies

Reduction

"I'm looking at that 3,000 [cm^{-1}] peak, and I'm having a hard time piecing together what it might be. I think it might be an alkane, but it's not like a big functional group that we talked about a lot, like anything that's really special."

Failed to recognize important spectral features and eliminated them as information to process

Common heuristics[7]

1. One-reason decision making
2. Rigidity
3. Generalization
4. Processing fluency
5. Associative activation
6. Affect
7. Representiveness
8. Reduction
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10. More A – More B

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Talanquer, 2014, *J. Chem. Ed*.

Results: Retrospective Think-aloud Interviews

Heuristic reasoning strategies

Affective Judgement:

"I chose yes because I guess that I feel like it was there in a small amount…. So I could redo the NMR with a higher concentration to see if it was what I thought it was or not. And so I just kind of had a gut feeling that it was there."

Participant felt positive about data

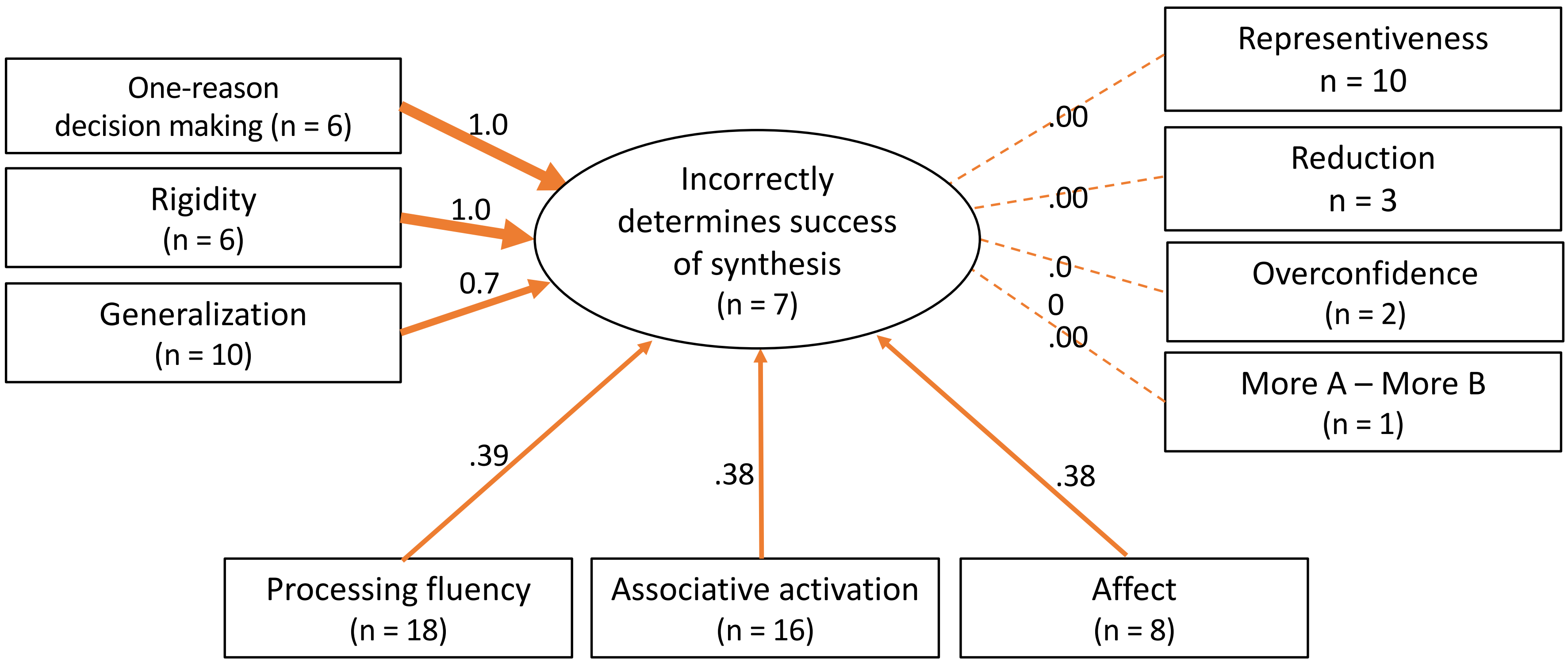
Common heuristics[7]

1. One-reason decision making
2. Rigidity
3. Generalization
4. Processing fluency
5. Associative activation
6. Affect
7. Representiveness
8. Reduction
9. Overconfidence
10. More A – More B

Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

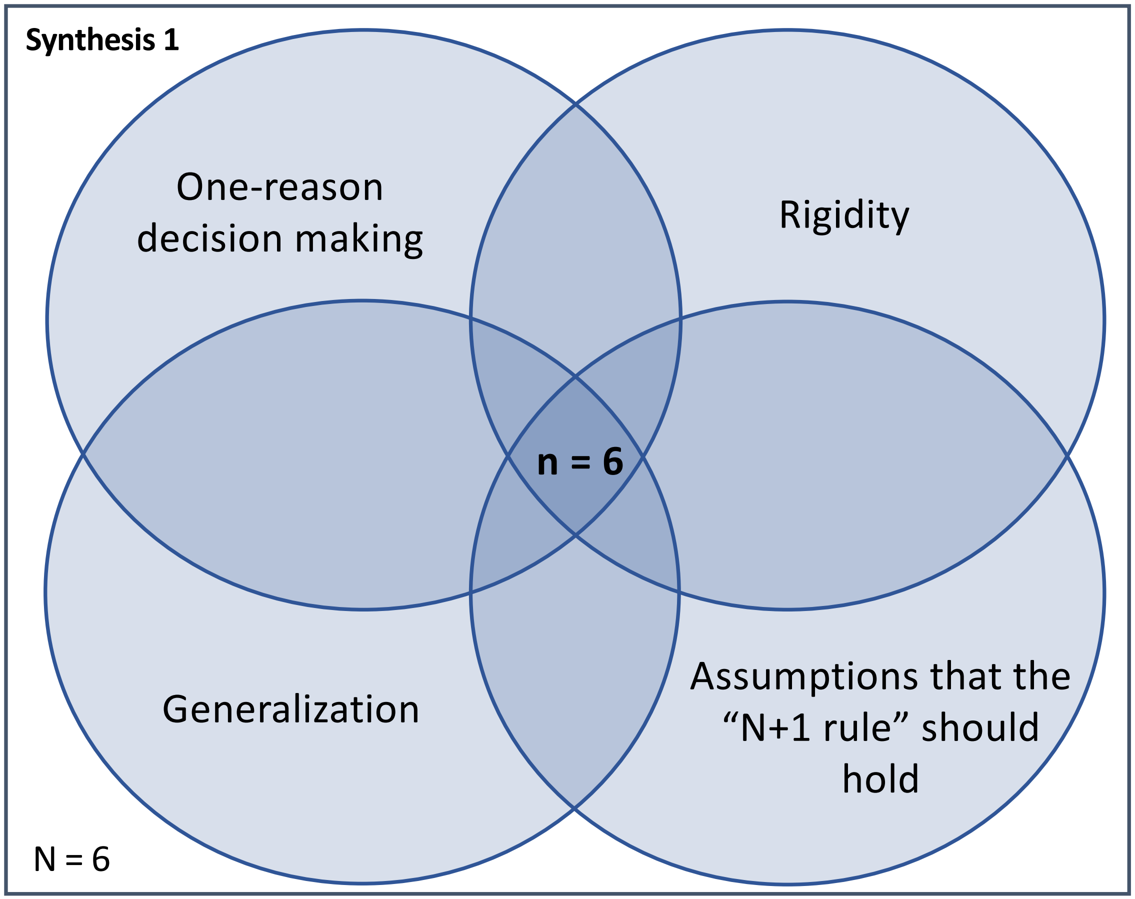
Talanquer, 2014, *J. Chem. Ed*.

Some heuristics are more problematic than others



Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Students who used multiple problematic heuristics were more likely to give an incorrect response



Connor, M.; Finkenstaedt-Quinn, S.; Shultz, G.V. Chem. Educ. Res. Pract. 2019, Advance Article

Summary

- Problematic reasoning among students is due to combination of their underlying assumptions and heuristics
- Students who successfully solved tasks evaluated spectral cues differently than those who didn't; Particular invalid chemical assumptions and heuristic reasoning strategies appear to constrain students' reasoning
- We have characterized productive reasoning strategies and valid assumptions and are collecting additional data with more experienced chemists

Connor, Megan C., Solaire A. Finkenstaedt-Quinn, and Ginger V. Shultz. "Constraints on organic chemistry students' reasoning during IR and 1 H NMR spectral interpretation." *Chemistry Education Research and Practice* (2019).

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