Supporting Information

Blooming Student Difficulties in Dealing with Organic Reaction Mechanisms – An Attempt at Systemization

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Supporting Information 1

Table 1: Coding scheme for classifying learning objectives and unachieved learning objectives into Bloom's revised taxonomy.

	Code	Code description (unachieved) learning objective includes…	Example
Knowledge dimension	*Factual knowledge*	basic knowledge elements that are content-related and are not connected with other knowledge elements, such as names of mechanisms, reactants or concepts, and fixed properties like atomic size or electronegativity values	*"I don't know the electronegativity of chlorine off the top of my head right now, nor that of carbon." (The students is not able to recall electronegativity values.)*
	Conceptual knowledge	complex knowledge elements that are content-related and connected and influence each other, such as organic reaction mechanisms, reactants or chemical concepts	*The students should be able to decide whether the reaction favors the Hofmann or Saytzeff product.*
	Procedural knowledge	knowledge of organic chemistry specific methods, algorithms, skills, techniques or criteria for applying a procedure, such as the steps that have to be completed to solve an organic reaction mechanisms, approaches for solving reaction mechanisms or knowledge of laboratory techniques	/
	Metacognitive knowledge	knowledge of cognition in general and the awareness one's own cognition, such learning strategies for learning organic reaction mechanisms or knowledge of which reaction mechanisms one has understood and which one has not	/
C	*Remember*	processes in which information is	*The students should be able to recall*

		retrieved from memory, such as definitions of chemical concepts or names of their properties	*properties that influence the difference between reaction A and B.*
	Understand	processes in which meaning is constructed from given information, such as translating representations into written or oral language, or classifying representations as specific reactants	*"So, it's an E2 elimination, tetrahydrofluoride is my base then." (The student is not able to classify the base.)*
	Apply	processes in which information is used in the context of a familiar or unfamiliar task, such as performing reaction steps or explaining how chemical concepts influence the task	*"And so I think that a CH_3 group will split off. And then, afterwards you have the nitrogen with chloride again." (The student is not able to produce the correct products based on the mechanism.)*
	Analyze	processes in which information is differentiated to determine similarities and differences and to distinguish relevant parts from irrelevant parts, such as identifying relevant parts of representations or distinguishing one chemical concept from another	*The students should be able to derive properties that differ between reaction A and B from the representation.*
o	*Evaluate*	processes in which information is checked and weighed against each other based on different criteria, such as checking and justifying one's own solution or comparing reactants on the basis of different criteria and making a decision	*The students should be able to compare and weigh influencing properties to decide which reaction proceeds faster.*

	Create	processes in which elements are reconstructed from an existing whole to form something new, such as planning a synthesis route	/

Supporting Information 2

Table 2: List of all content-related codes with examples covering the applied concepts.

Code	Sub code	Example
Mechanism	Elimination	*“Unlike E1 elimination, E2 elimination is synchronous.”*
	Nucleophilic substitution	*“This is a second-order nucleophilic substitution. Therefore, the chlorine leaves first as a chloride ion.”*
Reactant	Electrophile	*“Electrophilic means that it is positively charged, i.e. it is electron loving. In this sense, that would be the ether there with the chlorine at the end.”*
	Intermediate	*“Then the leaving group is removed and a cationic intermediate is formed […].”*
	Leaving group	*“So I initially assumed that the chloride was leaving as a leaving group, so to speak.”*
	Lewis base	*“[…] we have a sterically hindered base, which then tends to favor the more highly substituted product, i.e., the terminally eliminated product.”*
	Lewis acid	*“One explains bases and acids by saying that a base is an electron pair donor and an acid is an electron pair acceptor.”*
	Nucleophile	*“So generally you have a nucleophile, which is then also negatively charged.”*
	Product	*“I'm still not sure if my final product is even the right one.”*
	Solvent	*“We have the same solvent.”*
	Transition state	*“The transition state is stabilized by conjugation of the resulting negative charge.”*
Concept	Acidity	*“Because […] by the nucleophile from the chloride, I lower the electron density at the methyl rest […], so the CH acidity increases and it's deprotonable and/ Yes, exactly, that's why it's acidic now.”*
	Activation energy	*“Yes. So if I have a higher electronegativity, the reaction is more favorable, so my overall activation energy goes down, so to speak, the activation mountain is lower.”*
	Atomic radius	*“That was so that also the atomic radius had nevertheless also something to do with the polarizability.”*

	Basicity	*"Basicity is actually the ability to accept electrons."*
	Charge	*"The sulfur can attack because of its negative charge. This is because it is negatively charged. It has an excess of electrons and therefore wants to bind with its negative charge."*
	Electronegativity	*"I was just thinking about which element is more electronegative, sulfur or oxygen […]."*
	Electrophilicity	*"From the stability of the cation versus the electrophilicity of the rest there it is difficult to estimate, I would say, compared to the reaction before."*
	Hofmann/ Saytzeff	*"And sterically hindered bases tend to favor Hofmann, as far as I can remember, yes."*
	Hyperconjugation	*"Okay. Does the term `hyperconjugation' mean anything to you?" "No."*
	Inductive effect	*"So methyl groups or alkyl groups always have a +I-effect and this +I-effect means that they increase the electron density at the neighboring atom."*
	Leaving group ability	*"I could imagine that a high basicity also describes a poor leaving group, because the bond would then be or should be correspondingly weaker for a good leaving group."*
	Mesomeric effect	*"So I could imagine the mesomeric effect of bromine having an effect."*
	Nucleophilicity	*"The solvent has an effect on the nucleophilicity of the nucleophile."*
	Partial charge	*"We have a partial positive charge at the site of chlorine, at the carbon."*
	Polarizability	*"The polarizability thus determines how easily I can polarize a molecule. This depends largely on how high the charge density is. Firstly, on the charge and secondly on the size of the ion, the ion radius."*
	Reaction rate	*"That's why I would say that A proceeds faster, because the anion is less stable."*
	Resonance	*"Could you try to explain what resonance is?"* *"Yes, I have the same number of atoms, but a different structure."*

	Stability	*“I would say now it's stable because the N, the amine, has now reached the noble gas state.”*
	Steric hindrance	*“In the case of B, the nucleophile is sterically hindered due to branching, so attacking the backside is more difficult.”*
	Solvation	*“[…] that the resulting leaving group is stably solvated in the solvent, that it does not do another reaction, even if it is reactive.”*

Supporting Information 3

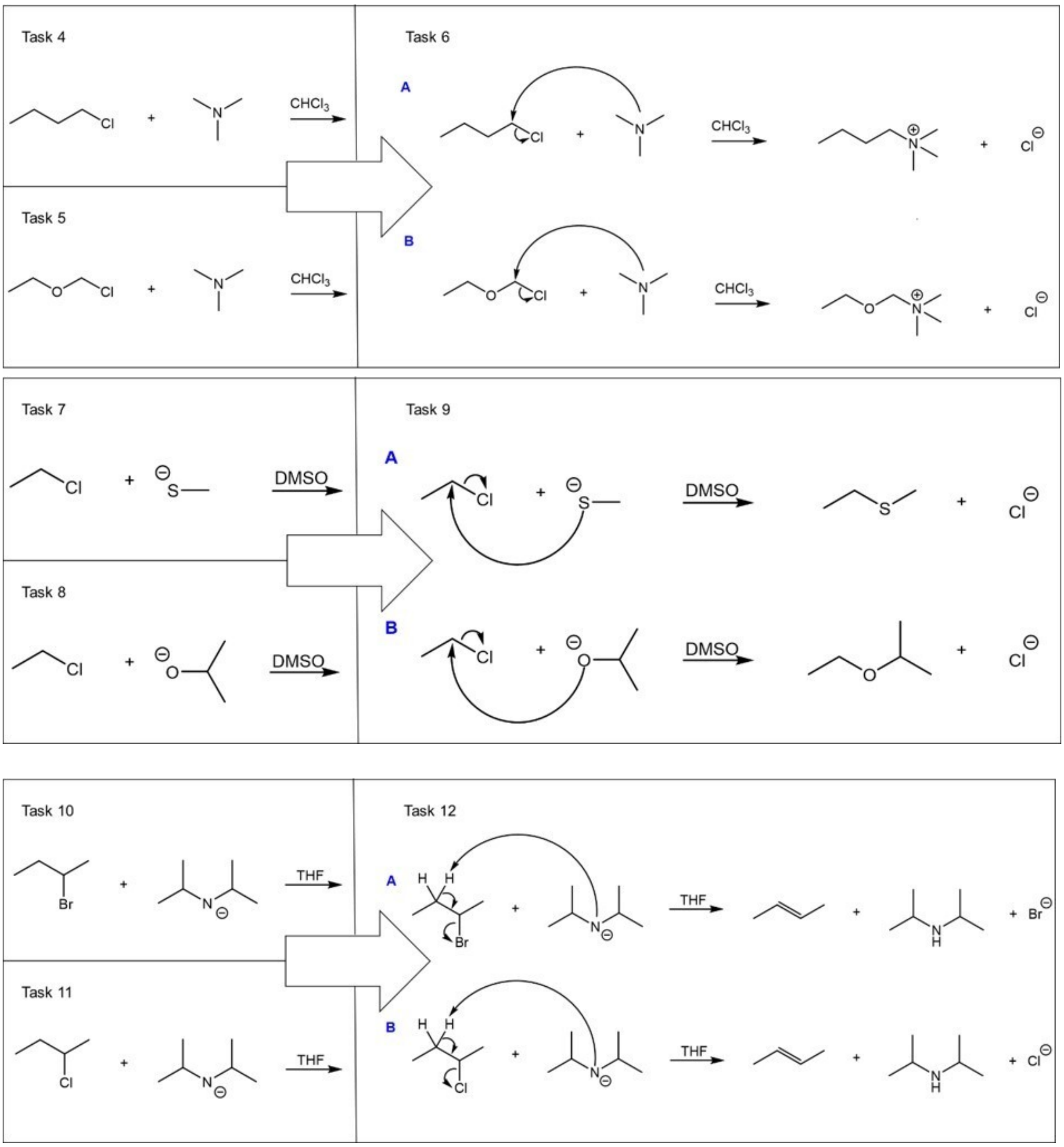

Figure 1: Overview of nucleophilic substitution and elimination tasks used in the study. The two predict-the-product tasks are shown on the left and the case comparison task is shown on the right.